Nonlinear differential equation problems

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Note: This note is still under development.

Contents

In a linear differential equation all terms involving the unknown fu
are linear in the unknown functions or their derivatives. Linear here mea
the unknown function or a derivative of it is multiplied by a number or a
function. All other differential equations are non-linear. The easiest way
an equation is nonlinear is to spot nonlinear terms where the unknown fu
or their derivatives are multiplied by each other. For example, in

$$u'(t) = -a(t)u(t) + b(t),$$

the terms involving the unknown function u are linear: u' contains the de
of the unknown function multiplied by unity, and au contains the u
function multiplied by a known function. However,

$$u'(t) = u(t)(1 - u(t)),$$

is nonlinear because of the term $-u^2$ where the unknown function is mu
by itself. Also

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0,$$

is nonlinear because of the term uu_x where the unknown function app
a product with itself or one if its derivatives. Another example of a no
equation is

$$u'' + \sin(u) = 0,$$

because $\sin(u)$ contains products of u,

$$\sin(u) = u - \frac{1}{3}u^3 + \ldots$$

A series of forthcoming examples will explain who to tackle nonlinea
ential equations with various techniques.

Introduction of basic concepts

onsider the (scaled) logistic equation

$$u'(t) = u(t)(1 - u(t))\,. \tag{1}$$

his is a nonlinear differential equation which will be solved by different strategies ı the following. A time discretization of (1) will either lead to a linear algebraic quation or a nonlinear algebraic equation at each time level. In the former ase, the time discretization method transforms the nonlinear ODE into linear ıbproblems at each time level, and the solution is straightforward to find nce linear algebraic equations are easy to solve by hand. However, when the me discretization leads to nonlinear algebraic equations, we cannot (except in ery rare cases) solve these without turning to approximate, iterative solution ıethods.

The following subsections first introduce various methods using (1):

- explicit time discretization methods (with no need to solve nonlinear algebraic equations)
- implicit Backward Euler discretization, leading to nonlinear algebraic equations solved by
  - an exact analytical technique
  - Picard iteration based on manual linearization
  - a single Picard step
  - Newton's method
- Implicit Crank-Nicolson discretization and linearization via a geometric mean formula

hereafter, we compare the performance of the various approaches. Despite the mplicity of (1), the conclusions reveal typical features of the various methods ı much more complicated nonlinear PDE problems.

.1 Linearization by explicit time discretization

Forward Euler method to solve (1) results in

$$\frac{u^{n+1} - u^n}{\Delta t} = u^n(1 - u^n),$$

hich is a *linear* algebraic equation for the unknown value u^{n+1}. The nonlinearity ı the original equation poses in this case no difficulty in the discrete algebraic quation. Any other explicit scheme in time will also give only linear algebraic quations to solve. For example, a typical 2nd-order Runge-Kutta method for .) reads,

$$u^* = u^n + \Delta t u^n(1 - u^n),$$
$$u^{n+1} = u^n + \Delta t \frac{1}{2}\left(u^n(1 - u^n) + u^*(1 - u^*)\right)\,.$$

The first step is linear in the unknown u^*. Then u^* is known in the ne which is linear in the unknown u^{n+1} .

1.2 Exact solution of nonlinear equations

Switching to a Backward Euler scheme for (1),

$$\frac{u^n - u^{n-1}}{\Delta t} = u^n(1 - u^n),$$

results in a nonlinear algebraic equation for the unknown value u^n. The e is of quadratic type:

$$\Delta t(u^n)^2 + (1 - \Delta t)u^n - u^{n-1} = 0\,.$$

We shall now introduce a shorter and often cleaner notation for nc algebraic equations at a given time level. The notation is inspired by the notation, i.e., variable names, used in a program, especially in more ac partial differential equation problems. The unknown in the algebraic equ denoted by u, while $u^{(1)}$ is the value of the unknown at the previous tir (in general $u^{(\ell)}$ is the value of the unknown ℓ levels back in time). The ı will be frequently used in later sections. What is meant by u (the exact of the PDE problem, the numerical approximation to the exact solution unknown solution at a certain time level) should be evident from the cc

The quadratic equation for the unknown u^n in (2) can with the new ı be written

$$F(u) = \Delta t u^2 + (1 - \Delta t)u - u^{(1)} = 0\,.$$

The solution is readily found to be

$$u = \frac{1}{2\Delta t}\left(-1 - \Delta t \pm \sqrt{(1 - \Delta t)^2 - 4\Delta t u^{(1)}}\right)\,.$$

Now we encounter a fundamental challenge with nonlinear algebraic eq the equation may have more than one solution. How do we pick the right s In the present simple case we can expand the square root in a series in truncate after the linear term since the Backward Euler scheme will in an error proportional to Δt anyway. Using `sympy` we find the following series expansions of the roots:

```
>>> import sympy as sp
>>> dt, u_1, u = sp.symbols('dt u_1 u')
>>> r1, r2 = sp.solve(dt*u**2 + (1-dt)*u - u_1, u)  # find roots
>>> r1
(dt - sqrt(dt**2 + 4*dt*u_1 - 2*dt + 1) - 1)/(2*dt)
>>> r2
(dt + sqrt(dt**2 + 4*dt*u_1 - 2*dt + 1) - 1)/(2*dt)
>>> print r1.series(dt, 0, 2)
-1/dt + 1 - u_1 + dt*(u_1**2 - u_1) + O(dt**2)
>>> print r2.series(dt, 0, 2)
u_1 + dt*(-u_1**2 + u_1) + O(dt**2)
```

We see that the `r1` root, corresponding to a minus sign in front of the square root in (4), behaves as $1/\Delta t$ and will therefore blow up as $\Delta t \to 0$! Therefore, only the `r2` root is of relevance in this case.

.3 Linearization

When the time integration of an ODE results in a nonlinear algebraic equation, we must normally find its solution by defining a sequence of linear equations and hope that the solutions of these linear equations converge to the desired solution of the nonlinear algebraic equation. Usually this means solving the linear equation repeatedly in an iterative fashion. Alternatively, the nonlinear equation can sometimes be approximated by one linear equation, and consequently there is no need for iteration.

Constructing a linear equation from a nonlinear one requires *linearization* of each nonlinear term. This can be done manually as in Picard iteration, or automatically algorithmically as in Newton's method. Examples will best illustrate how to linearize nonlinear problems.

.4 Picard iteration

Let us write (3) in a more compact form

$$F(u) = au^2 + bu + c = 0,$$

with $a = \Delta t$, $b = 1 - \Delta t$, and $c = -u^{(1)}$. Let u^- be an available approximation of the unknown u. Then we can linearize the term u^2 simply by writing $u^- u$. The resulting equation, $\hat{F}(u) = 0$, is now linear and hence easy to solve:

$$F(u) \approx \hat{F}(u) = au^- u + bu + c = 0\,.$$

Since the equation $\hat{F} = 0$ is only approximate, the solution u does not equal the exact solution u_e of the exact equation $F(u_\mathrm{e}) = 0$, but we can hope that u is closer to u_e than u^- is, and hence it makes sense to repeat the procedure, i.e., set $u^- = u$ and solve $\hat{F}(u) = 0$ again.

The idea of turning a nonlinear equation into a linear one by using an approximation u^- of u in nonlinear terms is a widely used approach that goes under many names: *fixed-point iteration*, the method of *successive substitutions*,

nonlinear Richardson iteration, and *Picard iteration*. We will stick to the name.

Picard iteration for solving the nonlinear equation arising from the Backward Euler discretization of the logistic equation can be written as

$$u = -\frac{c}{au^- + b}, \quad u^- \leftarrow u\,.$$

The iteration is started with the value of the unknown at the previous time level, $u^- = u^{(1)}$.

Some prefer an explicit iteration counter as superscript in the mathematical notation. Let u^k be the computed approximation to the solution in iteration k. In iteration $k+1$ we want to solve

$$au^k u^{k+1} + bu^{k+1} + c = 0 \quad \Rightarrow \quad u^{k+1} = -\frac{c}{au^k + b}, \quad k = 0, 1, \ldots$$

Since we need to perform the iteration at every time level, the time level counter is often also included:

$$au^{n+1,k}u^{n+1,k+1} + bu^{n+1,k+1} - u^n = 0 \quad \Rightarrow \quad u^{n+1,k+1} = \frac{u^n}{au^{n+1,k} + b},$$

with the start value $u^{n,0} = u^{n-1}$ and the final converged value $u^{n+1} = u^{n+1,k}$ for sufficiently large k.

However, we will normally apply a mathematical notation in our final formulas that is as close as possible to what we aim to write in a computer code, and then it becomes natural to use u and u^- instead of u^{k+1} and u^k or u^{n+1} and $u^{n+1,k}$.

Stopping criteria. The iteration method can typically be terminated when the change in the solution is smaller than a tolerance ϵ_u:

$$|u - u^-| \leq \epsilon_u,$$

or when the residual in the equation is sufficiently small (ϵ_r),

$$|F(u)| = |au^2 + bu + c| < \epsilon_r\,.$$

A single Picard iteration. Instead of iterating until a stopping criterion is fulfilled, one may iterate a specific number of times. Just one Picard iteration is popular as this corresponds to the intuitive idea of approximating a nonlinear term like $(u^n)^2$ by $u^{n-1}u^n$. This follows from the linearization $u^- u^n$ and the initial choice of $u^- = u^{n-1}$ at time level t_n. In other words, a single Picard iteration corresponds to using the solution at the previous time level to linearize nonlinear terms. The resulting discretization becomes

$$\frac{u^n - u^{n-1}}{\Delta t} = u^n(1 - u^{n-1}), \tag{5}$$

hich is a linear algebraic equation in the unknown u^n, and therefore we can asily solve for u^n, and there is no need for any alternative notation.

We shall later refer to the strategy of taking one Picard step, or equivalently, nearizing terms with use of the solution at the previous time step, as the *Picard1* ıethod. It is a widely used approach in science and technology, but with some mitations if Δt is not sufficiently small (as will be illustrated later).

Notice.

Equation (5) does not correspond to a "pure" finite difference method where the equation is sampled at a point and derivatives replaced by differences (because the u^{n-1} term on the right-hand side must then be u^n). The best interpretation of the scheme (5) is a Backward Euler difference combined with a single (perhaps insufficient) Picard iteration at each time level, with the value at the previous time level as start for the Picard iteration.

.5 Linearization by a geometric mean

Ve consider now a Crank-Nicolson discretization of (1). This means that the me derivative is approximated by a centered difference,

$$[D_t u = u(1-u)]^{n+\frac{1}{2}},$$

ritten out as

$$\frac{u^{n+1} - u^n}{\Delta t} = u^{n+\frac{1}{2}} - (u^{n+\frac{1}{2}})^2\,. \tag{6}$$

he term $u^{n+\frac{1}{2}}$ is normally approximated by an arithmetic mean,

$$u^{n+\frac{1}{2}} \approx \frac{1}{2}(u^n + u^{n+1}),$$

ıch that the scheme involves the unknown function only at the time levels where e actually compute it. The same arithmetic mean applied to the nonlinear ɛrm gives

$$(u^{n+\frac{1}{2}})^2 \approx \frac{1}{4}(u^n + u^{n+1})^2,$$

hich is nonlinear in the unknown u^{n+1}. However, using a *geometric mean* for $\iota^{n+\frac{1}{2}})^2$ is a way of linearizing the nonlinear term in (6):

$$(u^{n+\frac{1}{2}})^2 \approx u^n u^{n+1}\,.$$

Using an arithmetic mean on the linear $u^{n+\frac{1}{2}}$ term in (6) and a geometr for the second term, results in a linearized equation for the unknown u

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}(u^n + u^{n+1}) + u^n u^{n+1},$$

which can readily be solved:

$$u^{n+1} = \frac{1 + \frac{1}{2}\Delta t}{1 + \Delta t u^n - \frac{1}{2}\Delta t} u^n\,.$$

This scheme can be coded directly, and since there is no nonlinear a equation to iterate over, we skip the simplified notation with u for u $u^{(1)}$ for u^n. The technique with using a geometric average is an exa transforming a nonlinear algebraic equation to a linear one, without a for iterations.

The geometric mean approximation is often very effective for lin quadratic nonlinearities. Both the arithmetic and geometric mean app tions have truncation errors of order Δt^2 and are therefore compatible truncation error $\mathcal{O}(\Delta t)$ of the centered difference approximation for u Crank-Nicolson method.

Applying the operator notation for the means and finite differen linearized Crank-Nicolson scheme for the logistic equation can be co expressed as

$$[D_t u = \overline{u}^t + \overline{u^2}^{t,g}]^{n+\frac{1}{2}}\,.$$

Remark.

If we use an arithmetic instead of a geometric mean for the nonl term in (6), we end up with a nonlinear term $(u^{n+1})^2$. This term c linearized as $u^- u^{n+1}$ in a Picard iteration approach and in particul $u^n u^{n+1}$ in a Picard1 iteration approach. The latter gives a scheme al identical to the one arising from a geometric mean (the difference in being $\frac{1}{4}\Delta t u^n(u^{n+1} - u^n) \approx \frac{1}{4}\Delta t^2 u' u$, i.e., a difference of $\mathcal{O}(\Delta t^2)$).

1.6 Newton's method

The Backward Euler scheme (2) for the logistic equation leads to a n algebraic equation (3). Now we write any nonlinear algebraic equatio general and compact form

$$F(u) = 0\,.$$

Newton's method linearizes this equation by approximating $F(u)$ by it series expansion around a computed value u^- and keeping only the lin

$$F(u) = F(u^-) + F'(u^-)(u-u^-) + \frac{1}{2}F''(u^-)(u-u^-)^2 + \cdots$$
$$\approx F(u^-) + F'(u^-)(u-u^-) = \hat{F}(u)\,.$$

he linear equation $\hat{F}(u) = 0$ has the solution

$$u = u^- - \frac{F(u^-)}{F'(u^-)}\,.$$

xpressed with an iteration index in the unknown, Newton's method takes on
ıe more familiar mathematical form

$$u^{k+1} = u^k - \frac{F(u^k)}{F'(u^k)}, \quad k = 0, 1, \ldots$$

It can be shown that the error in iteration $k+1$ of Newton's method is the
quare of the error in iteration k, a result referred to as *quadratic convergence*.
his means that for small errors the method converges very fast, and in particular
ıuch faster than Picard iteration and other iteration methods. (The proof of
ıis result is found in most textbooks on numerical analysis.) However, the
uadratic convergence appears only if u^k is sufficiently close to the solution.
urther away from the solution the method can easily converge very slowly or
iverge. The reader is encouraged to do Exercise 3 to get a better understanding
ɔr the behavior of the method.

Application of Newton's method to the logistic equation discretized by the
ackward Euler method is straightforward as we have

$$F(u) = au^2 + bu + c, \quad a = \Delta t,\ b = 1 - \Delta t,\ c = -u^{(1)},$$

ıd then

$$F'(u) = 2au + b\,.$$

he iteration method becomes

$$u = u^- + \frac{a(u^-)^2 + bu^- + c}{2au^- + b}, \quad u^- \leftarrow u\,. \tag{7}$$

t each time level, we start the iteration by setting $u^- = u^{(1)}$. Stopping criteria
s listed for the Picard iteration can be used also for Newton's method.

An alternative mathematical form, where we write out a, b, and c, and use a
me level counter n and an iteration counter k, takes the form

$$^{n,k+1} = u^{n,k} + \frac{\Delta t(u^{n,k})^2 + (1-\Delta t)u^{n,k} - u^{n-1}}{2\Delta t u^{n,k} + 1 - \Delta t}, \quad u^{n,0} = u^{n-1}, \quad k = 0, 1, \ldots \tag{8}$$

. program implementation is much closer to (7) than to (8), but the latter is
etter aligned with the established mathematical notation used in the literature.

1.7 Relaxation

One iteration in Newton's method or Picard iteration consists of solving
problem $\hat{F}(u) = 0$. Sometimes convergence problems arise because t
solution u of $\hat{F}(u) = 0$ is "too far away" from the previously computed
u^-. A remedy is to introduce a relaxation, meaning that we first solve $\hat{F}($
for a suggested value u^* and then we take u as a weighted mean of what
u^-, and what our linearized equation $\hat{F} = 0$ suggests, u^*:

$$u = \omega u^* + (1-\omega)u^-\,.$$

The parameter ω is known as a *relaxation parameter*, and a choice $\omega <$
prevent divergent iterations.

Relaxation in Newton's method can be directly incorporated in tl
iteration formula:

$$u = u^- - \omega\frac{F(u^-)}{F'(u^-)}\,.$$

1.8 Implementation and experiments

The program `logistic.py`[1] contains implementations of all the metl
scribed above. Below is an extract of the file showing how the Picard and
methods are implemented for a Backward Euler discretization of the
equation.

```
def BE_logistic(u0, dt, Nt, choice='Picard',
                eps_r=1E-3, omega=1, max_iter=1000):
    if choice == 'Picard1':
        choice = 'Picard'
        max_iter = 1

    u = np.zeros(Nt+1)
    iterations = []
    u[0] = u0
    for n in range(1, Nt+1):
        a = dt
        b = 1 - dt
        c = -u[n-1]

        if choice == 'Picard':

            def F(u):
                return a*u**2 + b*u + c

            u_ = u[n-1]
            k = 0
            while abs(F(u_)) > eps_r and k < max_iter:
                u_ = omega*(-c/(a*u_ + b)) + (1-omega)*u_
                k += 1
            u[n] = u_
            iterations.append(k)
```

[1] `http://tinyurl.com/nm5587k/nonlin/logistic.py`

```
        elif choice == 'Newton':

            def F(u):
                return a*u**2 + b*u + c

            def dF(u):
                return 2*a*u + b

            u_ = u[n-1]
            k = 0
            while abs(F(u_)) > eps_r and k < max_iter:
                u_ = u_ - F(u_)/dF(u_)
                k += 1
            u[n] = u_
            iterations.append(k)
    return u, iterations
```

The Crank-Nicolson method utilizing a linearization based on the geometric ıean gives a simpler algorithm:

```
def CN_logistic(u0, dt, Nt):
    u = np.zeros(Nt+1)
    u[0] = u0
    for n in range(0, Nt):
        u[n+1] = (1 + 0.5*dt)/(1 + dt*u[n] - 0.5*dt)*u[n]
    return u
```

We may run experiments with the model problem (1) and the different ;rategies for dealing with nonlinearities as described above. For a quite coarse me resolution, $\Delta t = 0.9$, use of a tolerance $\epsilon_r = 0.1$ in the stopping criterion ıtroduces an iteration error, especially in the Picard iterations, that is visibly ıuch larger than the time discretization error due to a large Δt. This is lustrated by comparing the upper two plots in Figure 1. The one to the right as a stricter tolerance $\epsilon = 10^{-3}$, which leads to all the curves corresponding to icard and Newton iteration to be on top of each other (and no changes can be isually observed by reducing ϵ_r further). The reason why Newton's method does ıuch better than Picard iteration in the upper left plot is that Newton's method ith one step comes far below the ϵ_r tolerance, while the Picard iteration needs n average 7 iterations to bring the residual down to $\epsilon_r = 10^{-1}$, which gives ısufficient accuracy in the solution of the nonlinear equation. It is obvious that ıe Picard1 method gives significant errors in addition to the time discretization nless the time step is as small as in the lower right plot.

The *BE exact* curve corresponds to using the exact solution of the quadratic quation at each time level, so this curve is only affected by the Backward Euler me discretization. The *CN gm* curve corresponds to the theoretically more ccurate Crank-Nicolson discretization, combined with a geometric mean for nearization. This curve appear as more accurate, especially if we take the plot ı the lower right with a small Δt and an appropriately small ϵ_r value as the xact curve.

When it comes to the need for iterations, Figure 2 displays the number of erations required at each time level for Newton's method and Picard iteration.

The smaller Δt is, the better starting value we have for the iteration, faster the convergence is. With $\Delta t = 0.9$ Picard iteration requires on 32 iterations per time step, but this number is dramatically reduced a reduced.

However, introducing relaxation and a parameter $\omega = 0.8$ imm reduces the average of 32 to 7, indicating that for the large $\Delta t = 0.9$, iteration takes too long steps. An approximately optimal value for ω case is 0.5, which results in an average of only 2 iterations! Even more d impact of ω appears when $\Delta t = 1$: Picard iteration does not convergence iterations, but $\omega = 0.5$ again brings the average number of iterations do

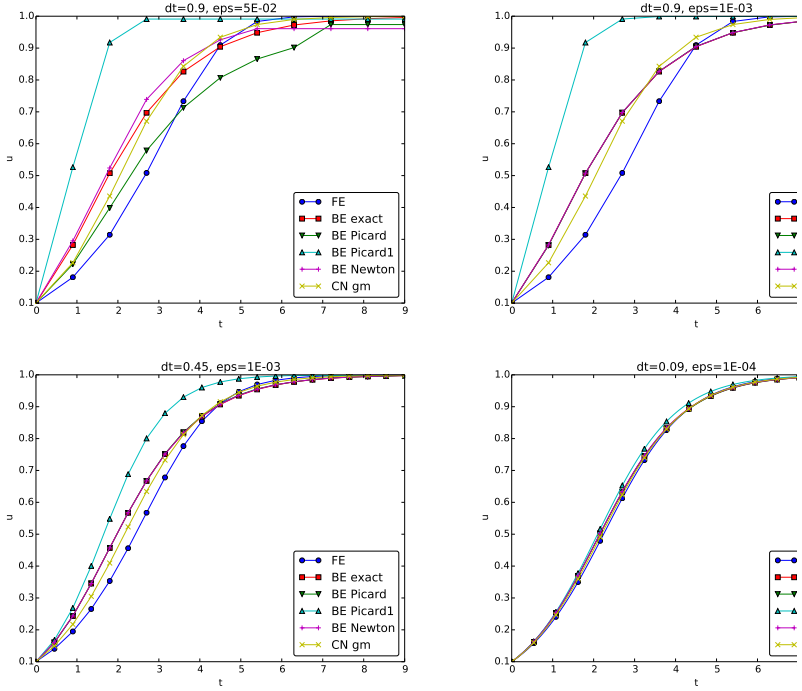
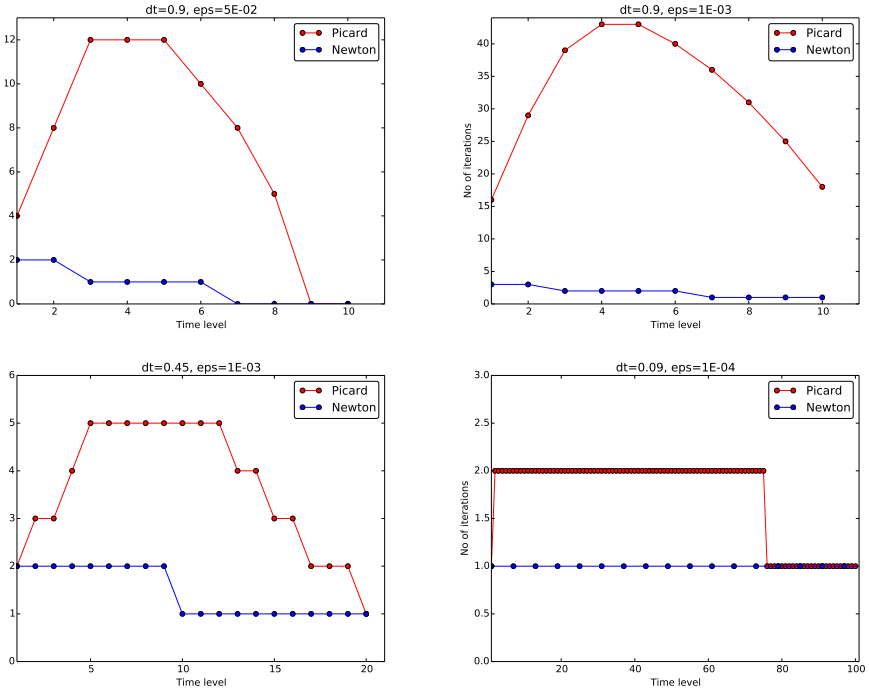


Figure 1: The impact of solution strategies and for four different ti lengths on the solution.

Experiments with this program reveal the relative performance of the ı as summarized in the table below. The Picard and Newton columns rel typical number of iterations with these methods before the curve starts t out and the number of iterations is significantly reduced since the solutio nonlinear algebraic equation is very close to the starting value for the it (the solution at the previous time level). Increasing Δt moves the startii further away from the solution of the nonlinear equation and one exp increase in the number of iterations. Picard iteration is very much more s



igure 2: Comparison of the number of iterations at various time levels for icard and Newton iteration.

› the size of Δt than Newton's method. The tolerance ϵ_r in residual-based :opping criterion takes on a low and high value in the experiments.

Δt	ϵ_r	Picard	Newton
0.2	10^{-7}	5	2
0.2	10^{-3}	2	1
0.4	10^{-7}	12	3
0.4	10^{-3}	4	2
0.8	10^{-7}	58	3
0.8	10^{-3}	4	2

:emark. The simple Crank-Nicolson method with a geometric mean for the uadratic nonlinearity gives visually more accurate solutions than the Backward uler discretization. Even with a tolerance of $\epsilon_r = 10^{-3}$, all the methods for eating the nonlinearities in the Backward Euler discretization gives graphs that annot be distinguished. So for accuracy in this problem, the time discretization much more crucial than ϵ_r. Ideally, one should estimate the error in the time iscretization, as the solution progresses, and set ϵ_r accordingly.

1.9 Generalization to a general nonlinear ODE

Let us see how the various methods in the previous sections can be ap the more generic model

$$u' = f(u, t),$$

where f is a nonlinear function of u.

Explicit time discretization. Explicit ODE methods like the Forwa scheme, Runge-Kutta methods, Adams-Bashforth methods all evalua time levels where u is already computed, so nonlinearities in f do not p difficulties.

Backward Euler discretization. Approximating u' by a backward di leads to a Backward Euler scheme, which can be written as

$$F(u^n) = u^n - \Delta t f(u^n, t_n) - u^{n-1} = 0,$$

or alternatively

$$F(u) = u - \Delta t f(u, t_n) - u^{(1)} = 0\,.$$

A simple Picard iteration, not knowing anything about the nonlinear st of f, must approximate $f(u, t_n)$ by $f(u^-, t_n)$:

$$\hat{F}(u) = u - \Delta t f(u^-, t_n) - u^{(1)}\,.$$

The iteration starts with $u^- = u^{(1)}$ and proceeds with repeating

$$u^* = \Delta t f(u^-, t_n) + u^{(1)}, \quad u = \omega u^* + (1-\omega)u^-, \quad u^- \leftarrow u,$$

until a stopping criterion is fulfilled.

Newton's method requires the computation of the derivative

$$F'(u) = 1 - \Delta t \frac{\partial f}{\partial u}(u, t_n)\,.$$

Starting with the solution at the previous time level, $u^- = u^{(1)}$, we can the standard formula

$$u = u^- - \omega \frac{F(u^-)}{F'(u^-)} = u^- - \omega \frac{u^{(1)} + \Delta t f(u^-, t_n)}{1 - \Delta t \frac{\partial}{\partial u} f(u^-, t_n)}\,.$$

The geometric mean trick cannot be used unless we know that f has a structure with quadratic expressions in u.

Crank-Nicolson discretization. The standard Crank-Nicolson scheme with rithmetic mean approximation of f takes the form

$$\frac{u^{n+1}-u^n}{\Delta t} = \frac{1}{2}(f(u^{n+1},t_{n+1}) + f(u^n,t_n))\,.$$

Ve can write the scheme as a nonlinear algebraic equation

$$F(u) = u - u^{(1)} - \Delta t\frac{1}{2}f(u,t_{n+1}) - \Delta t\frac{1}{2}f(u^{(1)},t_n) = 0\,. \tag{12}$$

Picard iteration scheme must in general employ the linearization,

$$\hat{F}(u) = u - u^{(1)} - \Delta t\frac{1}{2}f(u^-,t_{n+1}) - \Delta t\frac{1}{2}f(u^{(1)},t_n),$$

hile Newton's method can apply the general formula (11) with $F(u)$ given in .2) and

$$F'(u) = 1 - \frac{1}{2}\Delta t\frac{\partial f}{\partial u}(u,t_{n+1})\,.$$

Systems of nonlinear algebraic equations

nplicit time discretization methods for a system of ODEs, or a PDE, lead to *ystems* of nonlinear algebraic equations, written compactly as

$$F(u) = 0,$$

here u is a vector of unknowns $u = (u_0,\ldots,u_N)$, and F is a vector function: $' = (F_0,\ldots,F_N)$. Sometimes the equation system has a special structure ecause of the underlying problem, e.g.,

$$A(u)u = b(u),$$

ith $A(u)$ as an $(N+1)\times(N+1)$ matrix function of u and b as a vector function: $= (b_0,\ldots,b_N)$.

We shall next explain how Picard iteration and Newton's method can be pplied to systems like $F(u) = 0$ and $A(u)u = b(u)$. The exposition has a focus n ideas and practical computations. More theoretical considerations, including uite general results on convergence properties of these methods, can be found ı Kelley [1].

.1 Picard iteration

Ve cannot apply Picard iteration to nonlinear equations unless there is some pecial structure. For the commonly arising case $A(u)u = b(u)$ we can linearize ıe product $A(u)u$ to $A(u^-)u$ and $b(u)$ as $b(u^-)$. That is, we use the most reviously computed approximation in A and b to arrive at a *linear system* for :

$$A(u^-)u = b(u^-)\,.$$

A relaxed iteration takes the form

$$A(u^-)u^* = b(u^-), \quad u = \omega u^* + (1-\omega)u^-\,.$$

In other words, we solve a system of nonlinear algebraic equations as a s of linear systems.

Algorithm for relaxed Picard iteration.

Given $A(u)u = b(u)$ and an initial guess u^-, iterate until convergenc

1. solve $A(u^-)u^* = b(u^-)$ with respect to u^*
2. $u = \omega u^* + (1-\omega)u^-$
3. $u^- \leftarrow u$

2.2 Newton's method

The natural starting point for Newton's method is the general nonlinea equation $F(u) = 0$. As for a scalar equation, the idea is to approximate F a known value u^- by a linear function $\hat{F}$, calculated from the first two t a Taylor expansion of F. In the multi-variate case these two terms bec

$$F(u^-) + J(u^-)\cdot(u-u^-),$$

where J is the *Jacobian* of F, defined by

$$J_{i,j} = \frac{\partial F_i}{\partial u_j}\,.$$

So, the original nonlinear system is approximated by

$$\hat{F}(u) = F(u^-) + J(u^-)\cdot(u-u^-) = 0,$$

which is linear in u and can be solved in a two-step procedure: fir $J\delta u = -F(u^-)$ with respect to the vector δu and then update $u = u^-$ relaxation parameter can easily be incorporated:

$$u = \omega(u^- + \delta u) + (1-\omega)u^- = u^- + \omega\delta u\,.$$

Algorithm for Newton's method.

Given $F(u) = 0$ and an initial guess u^-, iterate until convergence:

1. solve $J\delta u = -F(u^-)$ with respect to δu
2. $u = u^- + \omega\delta u$
3. $u^- \leftarrow u$

For the special system with structure $A(u)u = b(u)$,

$$F_i = \sum_k A_{i,k}(u)u_k - b_i(u),$$

ne gets

$$J_{i,j} = \sum_k \frac{\partial A_{i,k}}{\partial u_j}u_k + A_{i,j} - \frac{\partial b_i}{\partial u_j}\,. \tag{13}$$

/e realize that the Jacobian needed in Newton's method consists of $A(u^-)$ as ı the Picard iteration plus two additional terms arising from the differentiation. sing the notation $A'(u)$ for $\partial A/\partial u$ (a quantity with three indices: $\partial A_{i,k}/\partial u_j$), nd $b'(u)$ for $\partial b/\partial u$ (a quantity with two indices: $\partial b_i/\partial u_j$), we can write the near system to be solved as

$$(A + A'u + b')\delta u = -Au + b,$$

r

$$(A(u^-) + A'(u^-)u^- + b'(u^-))\delta u = -A(u^-)u^- + b(u^-)\,.$$

earranging the terms demonstrates the difference from the system solved in ach Picard iteration:

$$\underbrace{A(u^-)(u^- + \delta u) - b(u^-)}_{\text{Picard system}} + \gamma(A'(u^-)u^- + b'(u^-))\delta u = 0\,.$$

ere we have inserted a parameter γ such that $\gamma = 0$ gives the Picard system nd $\gamma = 1$ gives the Newton system. Such a parameter can be handy in software o easily switch between the methods.

Combined algorithm for Picard and Newton iteration.

Given $A(u)$, $b(u)$, and an initial guess u^-, iterate until convergence:

1. solve $(A+\gamma(A'(u^-)u^-+b'(u^-)))\delta u = -A(u^-)u^-+b(u^-)$ with re to δu
2. $u = u^- + \omega\delta u$
3. $u^- \leftarrow u$

$\gamma = 1$ gives a Newton method while $\gamma = 0$ corresponds to Picard iterat

2.3 Stopping criteria

Let $||\cdot||$ be the standard Eucledian vector norm. Four termination crit much in use:

- Absolute change in solution: $||u - u^-|| \leq \epsilon_u$
- Relative change in solution: $||u - u^-|| \leq \epsilon_u||u_0||$, where u_0 den start value of u^- in the iteration
- Absolute residual: $||F(u)|| \leq \epsilon_r$
- Relative residual: $||F(u)|| \leq \epsilon_r||F(u_0)||$

To prevent divergent iterations to run forever, one terminates the it when the current number of iterations k exceeds a maximum value k_{ma}

The relative criteria are most used since they are not sensitive to t acteristic size of u. Nevertheless, the relative criteria can be misleadir the initial start value for the iteration is very close to the solution, s unnecessary reduction in the error measure is enforced. In such cases the a criteria work better. It is common to combine the absolute and relative n of the size of the residual, as in

$$||F(u)|| \leq \epsilon_{rr}||F(u_0)|| + \epsilon_{ra},$$

where ϵ_{rr} is the tolerance in the relative criterion and ϵ_{ra} is the toleranc absolute criterion. With a very good initial guess for the iteration (typic solution of a differential equation at the previous time level), the term | is small and ϵ_{ra} is the dominating tolerance. Otherwise, $\epsilon_{rr}||F(u_0)||$ relative criterion dominates.

With the change in solution as criterion we can formulate a combined a and relative measure of the change in the solution:

$$||\delta u|| \leq \epsilon_{ur}||u_0|| + \epsilon_{ua},$$

The ultimate termination criterion, combining the residual and the in solution with a test on the maximum number of iterations allow, expressed as

$$||F(u)|| \leq \epsilon_{rr}||F(u_0)|| + \epsilon_{ra} \quad \text{or} \quad ||\delta u|| \leq \epsilon_{ur}||u_0|| + \epsilon_{ua} \quad \text{or} \quad k > k_{\text{ma}}$$

.4 Example: A nonlinear ODE model from epidemiology

he simplest model spreading of a disease, such as a flu, takes the form of a × 2 ODE system

$$S' = -\beta SI, \tag{17}$$
$$I' = \beta SI - \nu I, \tag{18}$$

here $S(t)$ is the number of people who can get ill (susceptibles) and $I(t)$ is the umber of people who are ill (infected). The constants $\beta > 0$ and $\nu > 0$ must be iven along with initial conditions $S(0)$ and $I(0)$.

nplicit time discretization. A Crank-Nicolson scheme leads to a 2×2 ystem of nonlinear algebraic equations in the unknowns S^{n+1} and I^{n+1}:

$$\frac{S^{n+1} - S^n}{\Delta t} = -\beta[SI]^{n+\frac{1}{2}} \approx -\frac{\beta}{2}(S^n I^n + S^{n+1} I^{n+1}), \tag{19}$$
$$\frac{I^{n+1} - I^n}{\Delta t} = \beta[SI]^{n+\frac{1}{2}} - \nu I^{n+\frac{1}{2}} \approx \frac{\beta}{2}(S^n I^n + S^{n+1} I^{n+1}) - \frac{\nu}{2}(I^n + I^{n+1})\,. \tag{20}$$

ıtroducing S for S^{n+1}, $S^{(1)}$ for S^n, I for I^{n+1}, $I^{(1)}$ for I^n, we can rewrite the ystem as

$$F_S(S, I) = S - S^{(1)} + \frac{1}{2}\Delta t\beta(S^{(1)} I^{(1)} + SI) = 0, \tag{21}$$
$$F_I(S, I) = I - I^{(1)} - \frac{1}{2}\Delta t\beta(S^{(1)} I^{(1)} + SI) - \frac{1}{2}\Delta t\nu(I^{(1)} + I) = 0\,. \tag{22}$$

Picard iteration. We assume that we have approximations S_- and I_- to and I. A way of linearizing the only nonlinear term SI is to write $I_- S$ in ıe $F_S = 0$ equation and $S_- I$ in the $F_I = 0$ equation, which also *decouples* the quations. Solving the resulting linear equations with respect to the unknowns and I gives

$$S = \frac{S^{(1)} - \frac{1}{2}\Delta t\beta S^{(1)} I^{(1)}}{1 + \frac{1}{2}\Delta t\beta I_-},$$
$$I = \frac{I^{(1)} + \frac{1}{2}\Delta t\beta S^{(1)} I^{(1)}}{1 - \frac{1}{2}\Delta t\beta S_- + \nu}\,.$$

efore a new iteration, we must update $S^- \leftarrow S$ and $I^- \leftarrow I$.

Newton's method. The nonlinear system (21)-(22) can be written as 0 with $F = (F_S, F_I)$ and $u = (S, I)$. The Jacobian becomes

$$J = \begin{pmatrix} \frac{\partial}{\partial S}F_S & \frac{\partial}{\partial I}F_S \\ \frac{\partial}{\partial S}F_I & \frac{\partial}{\partial I}F_I \end{pmatrix} = \begin{pmatrix} 1 + \frac{1}{2}\Delta t\beta I & \frac{1}{2}\Delta t\beta \\ -\frac{1}{2}\Delta t\beta S & 1 - \frac{1}{2}\Delta t\beta I - \frac{1}{2}\Delta t\nu \end{pmatrix}$$

The Newton system $J(u^-)\delta u = -F(u^-)$ to be solved in each iteration

$$\begin{pmatrix} 1 + \frac{1}{2}\Delta t\beta I_- & \frac{1}{2}\Delta t\beta S_- \\ -\frac{1}{2}\Delta t\beta S_- & 1 - \frac{1}{2}\Delta t\beta I_- - \frac{1}{2}\Delta t\nu \end{pmatrix} \begin{pmatrix} \delta S \\ \delta I \end{pmatrix} = \begin{pmatrix} S_- - S^{(1)} + \frac{1}{2}\Delta t\beta(S^{(1)} I^{(1)} + S_- I_-) \\ I_- - I^{(1)} - \frac{1}{2}\Delta t\beta(S^{(1)} I^{(1)} + S_- I_-) - \frac{1}{2}\Delta t\nu(I^{(1)} + I_-) \end{pmatrix}$$

Remark. For this particular system of ODEs, explicit time integration ı work very well. The 4-th order Runge-Kutta method is an excellent between high accuracy, high efficiency, and simplicity.

3 Linearization at the differential equation

The attention is now turned to nonlinear partial differential equations and application of the techniques explained above for ODEs. The model] is a nonlinear diffusion equation

$$\frac{\partial u}{\partial t} = \nabla \cdot (\alpha(u)\nabla u) + f(u), \qquad \boldsymbol{x} \in \Omega,\ t \in (0, T],$$
$$-\alpha(u)\frac{\partial u}{\partial n} = g, \qquad \boldsymbol{x} \in \partial\Omega_N,\ t \in (0, T],$$
$$u = u_0, \qquad \boldsymbol{x} \in \partial\Omega_D,\ t \in (0, T]\,.$$

Our aim is to discretize the problem in time and then present tec for linearizing the time-discrete PDE problem "at the PDE level" su we transform the nonlinear stationary PDE problems at each time leve sequence of linear PDE problems, which can be solved using any met linear PDEs. This strategy avoids the solution systems of nonlinear a equations. In Section 4 we shall take the opposite (and more common) a discretize the nonlinear problem in time and space first, and then s resulting nonlinear algebraic equations at each time level by the met Section 2.

.1 Explicit time integration

he nonlinearities in the PDE are trivial to deal with if we choose an explicit me integration method for (23), such as the Forward Euler method:

$$[D_t^+ u = \nabla \cdot (\alpha(u)\nabla u) + f(u)]^n,$$

r written out,

$$\frac{u^{n+1} - u^n}{\Delta t} = \nabla \cdot (\alpha(u^n)\nabla u^n) + f(u^n),$$

hich is a linear equation in the unknown u^{n+1} with solution

$$u^{n+1} = u^n + \Delta t \nabla \cdot (\alpha(u^n)\nabla u^n) + \Delta t f(u^n)\,.$$

The disadvantage with this discretization is usually thought to be the stability iterion

$$\Delta t \leq \frac{1}{\max \alpha}(\Delta x^2 + \Delta y^2 + \Delta z^2),$$

or the case $f = 0$ and a standard 2nd-order finite difference discretization in pace with mesh cell sizes Δx, Δy, and Δz in the various spatial directions.

.2 Backward Euler scheme and Picard iteration

Backward Euler scheme for (23) reads

$$[D_t^- u = \nabla \cdot (\alpha(u)\nabla u) + f(u)]^n\,.$$

Written out,

$$\frac{u^n - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^n)\nabla u^n) + f(u^n)\,. \tag{26}$$

his is a nonlinear, stationary PDE for the unknown function $u^n(\boldsymbol{x})$. We troduce a Picard iteration with k as iteration counter. A typical linearization f the $\nabla \cdot \alpha(u^n)\nabla u^n$ term in iteration $k+1$ is to use the previously computed ^{n,k} approximation in the diffusion coefficient: $\alpha(u^{n,k})$. The nonlinear source erm is treated similarly: $f(u^{n,k})$. The unknown function $u^{n,k+1}$ then fulfills the near PDE

$$\frac{u^{n,k+1} - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^{n,k})\nabla u^{n,k+1}) + f(u^{n,k})\,. \tag{27}$$

he initial guess for the Picard iteration at this time level can be taken as the olution at the previous time level: $u^{n,0} = u^{n-1}$.

We can alternatively apply the implementation-friendly notation where u orresponds to the unknown we want to solve for, i.e., $u^{n,k+1}$ above, and u^- the most recently computed value, $u^{n,k}$ above. Moreover, $u^{(1)}$ denotes the

unknown function at the previous time level, u^{n-1} above. The PDE to b in a Picard iteration then looks like

$$\frac{u - u^{(1)}}{\Delta t} = \nabla \cdot (\alpha(u^-)\nabla u) + f(u^-)\,.$$

At the beginning of the iteration we start with the value from the previc level: $u^- = u^{(1)}$, and after each iteration, u^- is updated to u.

3.3 Backward Euler scheme and Newton's method

At time level n we have to solve the stationary PDE (26), this time with N method. Normally, Newton's method is defined for systems of *algebraic eq* but the idea of the method can be applied at the PDE level too.

Linearization via Taylor expansions. Let $u^{n,k}$ be an approximatio unknown u^n. We seek a better approximation on the form

$$u^n = u^{n,k} + \delta u\,.$$

The idea is to insert (29) in (26), Taylor expand the nonlinearities a keep the terms that are linear in δu. Then we can solve a linear PDE correction δu and use (29) to find a new approximation $u^{n,k+1} = u^{n,k}$ u^n.

Inserting (29) in (26) gives

$$\frac{u^{n,k} + \delta u - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^{n,k} + \delta u)\nabla(u^{n,k} + \delta u)) + f(u^{n,k} + \delta u)$$

We can Taylor expand $\alpha(u^{n,k} + \delta u)$ and $f(u^{n,k} + \delta u)$:

$$\alpha(u^{n,k} + \delta u) = \alpha(u^{n,k}) + \frac{d\alpha}{du}(u^{n,k})\delta u + \mathcal{O}(\delta u^2) \approx \alpha(u^{n,k}) + \alpha'(u^{n,k}$$
$$f(u^{n,k} + \delta u) = f(u^{n,k}) + \frac{df}{du}(u^{n,k})\delta u + \mathcal{O}(\delta u^2) \approx f(u^{n,k}) + f'(u^{n,k}$$

Inserting the linear approximations of α and f in (30) results in

$$\begin{aligned}\frac{u^{n,k} + \delta u - u^{n-1}}{\Delta t} = {} & \nabla \cdot (\alpha(u^{n,k})\nabla u^{n,k}) + f(u^{m,k}) + \\ & \nabla \cdot (\alpha(u^{n,k})\nabla \delta u) + \nabla \cdot (\alpha'(u^{n,k})\delta u \nabla u^{n,k}) + \\ & \nabla \cdot (\alpha'(u^{n,k})\delta u \nabla \delta u) + f'(u^{n,k})\delta u\end{aligned}$$

The term $\alpha'(u^{n,k})\delta u \nabla \delta u$ is $\mathcal{O}(\delta u^2)$ and therefore omitted. Reorganiz equation gives a PDE for δu that we can write in short form as

$$\delta F(\delta u; u^{n,k}) = -F(u^{n,k}),$$

here

$$F(u^{n,k}) = \frac{u^{n,k} - u^{n-1}}{\Delta t} - \nabla\cdot(\alpha(u^{n,k})\nabla u^{n,k}) + f(u^{n,k}), \tag{32}$$

$$\delta F(\delta u; u^{n,k}) = -\frac{1}{\Delta t}\delta u + \nabla\cdot(\alpha(u^{n,k})\nabla\delta u) + \nabla\cdot(\alpha'(u^{n,k})\delta u\nabla u^{n,k}) + f'(u^{n,k})\delta u\,. \tag{33}$$

ote that δF is a linear function of δu, and F contains only terms that are nown, such that the PDE for δu is indeed linear.

Observations.

The notational form $\delta F = -F$ resembles the Newton system $J\delta u = -F$ for systems of algebraic equations, with δF as $J\delta u$. The unknown vector in a linear system of algebraic equations enters the system as a linear operator in terms of a matrix-vector product ($J\delta u$), while at the PDE level we have a linear differential operator instead (δF).

imilarity with Picard iteration. We can rewrite the PDE for δu in a ightly different way too if we define $u^{n,k} + \delta u$ as $u^{n,k+1}$.

$$\frac{u^{n,k+1} - u^{n-1}}{\Delta t} = \nabla\cdot(\alpha(u^{n,k})\nabla u^{n,k+1}) + f(u^{n,k}) + \nabla\cdot(\alpha'(u^{n,k})\delta u\nabla u^{n,k}) + f'(u^{n,k})\delta u\,. \tag{34}$$

ote that the first line is the same PDE as arise in the Picard iteration, while the emaining terms arise from the differentiations that are an inherent ingredient ı Newton's method.

mplementation. For coding we want to introduce u for u^n, u^- for $u^{n,k}$ and $^{(1)}$ for u^{n-1}. The formulas for F and δF are then more clearly written as

$$F(u^-) = \frac{u^- - u^{(1)}}{\Delta t} - \nabla\cdot(\alpha(u^-)\nabla u^-) + f(u^-), \tag{35}$$

$$\delta F(\delta u; u^-) = -\frac{1}{\Delta t}\delta u + \nabla\cdot(\alpha(u^-)\nabla\delta u) + \nabla\cdot(\alpha'(u^-)\delta u\nabla u^-) + f'(u^-)\delta u\,. \tag{36}$$

The form that orders the PDE as the Picard iteration terms plus the method's derivative terms becomes

$$\frac{u - u^{(1)}}{\Delta t} = \nabla\cdot(\alpha(u^-)\nabla u) + f(u^-) + \gamma(\nabla\cdot(\alpha'(u^-)(u-u^-)\nabla u^-) + f'(u^-)(u-u^-))\,.$$

The Picard and full Newton versions correspond to $\gamma = 0$ and $\gamma = 1$, resp

3.4 Crank-Nicolson discretization

A Crank-Nicolson discretization of (23) applies a centered difference at

$$[D_t u = \nabla\cdot(\alpha(u)\nabla u) + f(u)]^{n+\frac{1}{2}}\,.$$

Since u is not known at $t_{n+\frac{1}{2}}$ we need to express the terms on the right-h via unknowns u^n and u^{n+1}. The standard technique is to apply an ari average,

$$u^{n+\frac{1}{2}} \approx \frac{1}{2}(u^n + u^{n+1})\,.$$

However, with nonlinear terms we have many choices of formulating an ari mean:

$$[f(u)]^{n+\frac{1}{2}} \approx f(\frac{1}{2}(u^n + u^{n+1})) = [f(\overline{u}^t)]^{n+\frac{1}{2}},$$

$$[f(u)]^{n+\frac{1}{2}} \approx frac12(f(u^n) + f(u^{n+1})) = [\overline{f(u)}^t]^{n+\frac{1}{2}},$$

$$[\alpha(u)\nabla u]^{n+\frac{1}{2}} \approx \alpha(\frac{1}{2}(u^n + u^{n+1}))\nabla(\frac{1}{2}(u^n + u^{n+1})) = \alpha(\overline{u}^t)\nabla\overline{u}^t]^{n+\frac{1}{2}},$$

$$[\alpha(u)\nabla u]^{n+\frac{1}{2}} \approx \frac{1}{2}(\alpha(u^n) + \alpha(u^{n+1}))\nabla(\frac{1}{2}(u^n + u^{n+1})) = [\overline{\alpha(u)}^t\nabla\overline{u}^t]^{n+}$$

$$[\alpha(u)\nabla u]^{n+\frac{1}{2}} \approx \frac{1}{2}(\alpha(u^n)\nabla u^n + \alpha(u^{n+1})\nabla u^{n+1}) = [\overline{\alpha(u)\nabla u}^t]^{n+\frac{1}{2}}\,.$$

4 Discretization of stationary nonlinear diff tial equations

Section 3 presents methods for linearizing time-discrete PDEs directly discretization in space. We can alternatively carry out the discretization and of the time-discrete nonlinear PDE problem and get a system of n algebraic equations, which can be solved by Picard iteration or Newton's as presented in Section 2. This latter approach will now be described i

We shall work with the 1D problem

$$-(\alpha(u)u')' + au = f(u), \quad x \in (0,L), \quad \alpha(u(0))u'(0) = C,\ u(L) = D\,. \quad (43)$$

his problem is of the same nature as those arising from implicit time integration f a nonlinear diffusion PDE as outlined in Section 3.2 (set $a = 1/\Delta t$ and let (u) incorporate the nonlinear source term as well as known terms with the me-dependent unknown function at the previous time level).

.1 Finite difference discretizations

he nonlinearity in the differential equation (43) poses no more difficulty than a ariable coefficient, as in $(\alpha(x)u')'$. We can therefore use a standard approach o discretizing the Laplace term with a variable coefficient:

$$[-D_x\alpha D_x u + au = f]_i\,.$$

/riting this out for a uniform mesh with points $x_i = i\Delta x$, $i = 0, \ldots, N_x$, leads o

$$-\frac{1}{\Delta x^2}\left(\alpha_{i+\frac{1}{2}}(u_{i+1} - u_i) - \alpha_{i-\frac{1}{2}}(u_i - u_{i-1})\right) + au_i = f(u_i)\,. \quad (44)$$

his equation is valid at all the mesh points $i = 0, 1, \ldots, N_x - 1$. At $i = N_x$ e have the Dirichlet condition $u_i = 0$. The only difference from the case with $\alpha(x)u')'$ and $f(x)$ is that now α and f are functions of u and not only on x: $\alpha(u(x))u')'$ and $f(u(x))$.

The quantity $\alpha_{i+\frac{1}{2}}$, evaluated between two mesh points, needs a comment. ince α depends on u and u is only known at the mesh points, we need to express $_{i+\frac{1}{2}}$ in terms of u_i and u_{i+1}. For this purpose we use an arithmetic mean, lthough a harmonic mean is also common in this context if α features large mps. There are two choices of arithmetic means:

$$\alpha_{i+\frac{1}{2}} \approx \alpha(\frac{1}{2}(u_i + u_{i+1}) = [\alpha(\overline{u}^x)]^{i+\frac{1}{2}}, \quad (45)$$

$$\alpha_{i+\frac{1}{2}} \approx \frac{1}{2}(\alpha(u_i) + \alpha(u_{i+1})) = [\overline{\alpha(u)}^x]^{i+\frac{1}{2}} \quad (46)$$

quation (44) with the latter approximation then looks like

$$-\frac{1}{2\Delta x^2}\left((\alpha(u_i) + \alpha(u_{i+1}))(u_{i+1} - u_i) - (\alpha(u_{i-1}) + \alpha(u_i))(u_i - u_{i-1})\right) + au_i = f(u_i), \quad (47)$$

r written more compactly,

$$[-D_x\overline{\alpha}^x D_x u + au = f]_i\,.$$

At mesh point $i = 0$ we have the boundary condition $\alpha(u)u' = C$, discretized by

$$[\alpha(u)D_{2x}u = C]_0,$$

meaning

$$\alpha(u_0)\frac{u_1 - u_{-1}}{2\Delta x} = C\,.$$

The fictitious value u_{-1} can be eliminated with the aid of (47) for $i = 0$. F (47) should be solved with respect to u_{i-1} and that value (for $i = 0$) sh inserted in (48), but it is algebraically much easier to do it the other way Alternatively, one can use a ghost cell $[-\Delta x, 0]$ and update the u_{-1} the ghost cell according to (48) after every Picard or Newton iteratio an approach means that we use a known u_{-1} value in (47) from the p iteration.

4.2 Solution of algebraic equations

The structure of the equation system. The nonlinear algebraic ec (47) are of the form $A(u)u = b(u)$ with

$$A_{i,i} = \frac{1}{2\Delta x^2}(-\alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a,$$
$$A_{i,i-1} = -\frac{1}{2\Delta x^2}(\alpha(u_{i-1}) + \alpha(u_i)),$$
$$A_{i,i+1} = -\frac{1}{2\Delta x^2}(\alpha(u_i) + \alpha(u_{i+1})),$$
$$b_i = f(u_i)\,.$$

The matrix $A(u)$ is tridiagonal: $A_{i,j} = 0$ for $j > 1 + 1$ and $j < i - 1$.

The above expressions are valid for internal mesh points $1 \leq i \leq N_x$ $i = 0$ we need to express $u_{i-1} = u_{-1}$ in terms of u_1 using (48):

$$u_{-1} = u_1 - \frac{2\Delta x}{\alpha(u_0)}\,.$$

This value must be inserted in $A_{0,0}$. The expression for $A_{i,i+1}$ applies f and $A_{i,i-1}$ does not enter the system when $i = 0$.

Regarding the last equation, its form depends on whether we incl Dirichlet condition $u(L) = D$, meaning $u_{N_x} = D$, in the nonlinear a equation system or not. Suppose we choose $(u_0, u_1, \ldots, u_{N_x-1})$ as un later referred to as *equations without Dirichlet conditions*. The last equa responds to $i = N_x - 1$. It involves the boundary value u_{N_x}, which is sub by D. If the unknown vector includes the boundary value, $(u_0, u_1, .$ later referred to as *equations including Dirichlet conditions*, the equa $i = N_x - 1$ just involves the unknown u_{N_x}, and the final equation l $u_{N_x} = D$, corresponding to $A_{i,i} = 1$ and $b_i = D$ for $i = N_x$.

icard iteration. The obvious Picard iteration scheme is to use previously omputed values of u_i in $A(u)$ and $b(u)$, as described more in detail in Section 2. The system $F(u) = 0$ is then solved with respect to u, where $F = (F_0, F_1, \ldots, F_m)$, $u = (u_0, u_1, \ldots, u_m)$, and the F_i expression is given above. The ndex m is N_x in equations including the Dirichlet condition and $N_x - 1$ when ne Dirichlet condition is excluded.

To write out the mathematical details, we introduce u^- as the most recent pproximation to solution vector u, and u_i^- is the i-th component in u, which is ne most recently computed value of the unknown u_i. For the case $N_x = 2$ we et the following system to solve in case we omit the Dirichlet condition from ne system:

$$\begin{pmatrix} \frac{1}{2\Delta x^2}(-\alpha(u_1^-) + 2\alpha(u_0^-) - \alpha(u_1^-)) + a & -\frac{1}{2\Delta x^2}(\alpha(u_0^-) + \alpha(u_1^-)) \\ -\frac{1}{2\Delta x^2}(\alpha(u_0^-) + \alpha(u_1^-)) & \frac{1}{2\Delta x^2}(-\alpha(u_0^-) + 2\alpha(u_1^-) - \alpha(u_2)) + a \end{pmatrix} \begin{pmatrix}$$

here u_{-1} must be substituted by (49), and u_2 by D.

The system with the Dirichlet condition becomes

$$\begin{pmatrix} \frac{1}{2\Delta x^2}(-\alpha(u_1^-) + 2\alpha(u_0^-) - \alpha(u_1^-)) + a & 0 \\ -\frac{1}{2\Delta x^2}(\alpha(u_0^-) + \alpha(u_1^-)) & \\ -\frac{1}{2\Delta x^2}(\alpha(u_0^-) + \alpha(u_1^-)) & \frac{1}{2\Delta x^2}(-\alpha(u_0^-) + 2\alpha(u_1^-) - \alpha(u_2)) + a \\ 0 & 0 \end{pmatrix} -$$

Newton's method. The Jacobian must be derived in order to use Newton's ethod. Here it means that we need to differentiate $F(u) = A(u)u - b(u)$ with espect to the unknown parameters $u_0, u_1, \ldots, u_m$ ($m = N_x$ or $m = N_x - 1$, epending on whether the Dirichlet condition is included in the nonlinear system $(u) = 0$ or not). Nonlinear equation number i has the structure

$$_i = A_{i,i-1}(u_{i-1}, u_i)u_{i-1} + A_{i,i}(u_{i-1}, u_i, u_{i+1})u_i + A_{i,i+1}(u_i, u_{i+1})u_{i+1} - b_i(u_i)\,.$$

omputing the Jacobian requires careful differentiation. For example,

$$\begin{aligned} \frac{\partial}{\partial u_i}(A_{i,i}(u_{i-1}, u_i, u_{i+1})u_i) &= \frac{\partial A_{i,i}}{\partial u_i}u_i + A_{i,i}\frac{\partial u_i}{\partial u_i} \\ &= \frac{\partial}{\partial u_i}(\frac{1}{2\Delta x^2}(-\alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a)u_i + \\ &\quad \frac{1}{2\Delta x^2}(-\alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a) \\ &= \frac{1}{2\Delta x^2}(2\alpha'(u_i)u_i - \alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a\,. \end{aligned}$$

he complete Jacobian becomes

$$\begin{aligned} J_{i,i} &= \frac{\partial F_i}{\partial u_i} = \frac{\partial A_{i,i-1}}{\partial u_i}u_{i-1} + \frac{\partial A_{i,i}}{\partial u_i}u_i + A_{i,i} + \frac{\partial A_{i,i+1}}{\partial u_i}u_{i+1} - \frac{\partial b_i}{\partial u_i} \\ &= \frac{1}{2\Delta x^2}(-\alpha'(u_i)u_{i-1} + 2\alpha'(u_i)u_i - \alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+} \\ &\quad a - \frac{1}{2\Delta x^2}\alpha'(u_i)u_{i+1} - b'(u_i), \\ J_{i,i-1} &= \frac{\partial F_i}{\partial u_{i-1}} = \frac{\partial A_{i,i-1}}{\partial u_{i-1}}u_{i-1} + A_{i-1,i} + \frac{\partial A_{i,i}}{\partial u_{i-1}}u_i - \frac{\partial b_i}{\partial u_{i-1}} \\ &= \frac{1}{2\Delta x^2}(-\alpha'(u_{i-1})u_{i-1} - (\alpha(u_{i-1}) + \alpha(u_i)) + \alpha'(u_{i-1})u_i), \\ J_{i,i+1} &= \frac{\partial A_{i,i+1}}{\partial u_{i-1}}u_{i+1} + A_{i+1,i} + \frac{\partial A_{i,i}}{\partial u_{i+1}}u_i - \frac{\partial b_i}{\partial u_{i+1}} \\ &= \frac{1}{2\Delta x^2}(-\alpha'(u_{i+1})u_{i+1} - (\alpha(u_i) + \alpha(u_{i+1})) + \alpha'(u_{i+1})u_i)\,. \end{aligned}$$

The explicit expression for nonlinear equation number i, $F_i(u_0, u_1, \ldots$ from moving the (u_i) term in (47) to the left-hand side:

$$\begin{aligned} F_i = & = -\frac{1}{2\Delta x^2}\left((\alpha(u_i) + \alpha(u_{i+1}))(u_{i+1} - u\right. \\ & + au_i - f(u_i) = 0\,. \end{aligned}$$

At the boundary point $i = 0$, u_{-1} must be replaced using the formu When the Dirichlet condition at $i = N_x$ is not a part of the equation the last equation $F_m = 0$ for $m = N_x - 1$ involves the quantity u_{N_x}– must be replaced by D. If u_{N_x} is treated as an unknown in the system, equation $F_m = 0$ has $m = N_x$ and reads

$$F_{N_x}(u_0, \ldots, u_{N_x}) = u_{N_x} - D = 0\,.$$

Similar replacement of u_{-1} and u_{N_x} must be done in the Jacobian for and last row. When u_{N_x} is included as an unknown, the last row in the J must help implement the condition $\delta u_{N_x} = 0$, since we assume that u the right Dirichlet value at the beginning of the iteration ($u_{N_x} = D$), a the Newton update should be zero for $i = 0$, i.e., $\delta u_{N_x} = 0$. This also fo right-hand side to be $b_i = 0$, $i = N_x$.

We have seen, and can see from the present example, that the linear in Newton's method contains all the terms present in the system tha in the Picard iteration method. The extra terms in Newton's method multiplied by a factor such that it is easy to program one linear system this factor to 0 or 1 to generate the Picard or Newton system.

4.3 Galerkin-type discretizations

For the finite element discretization we first need to derive the var problem. Let V be an appropriate function space with basis functions {

ecause of the Dirichlet condition at $x = L$ we require $\psi_i(L) = 0$, $i \in \mathcal{I}_s$. The pproximate solution is written as $u = D + \sum_{j\in\mathcal{I}_s} c_j\psi_j$, where the term D can e viewed as a boundary function needed to implement the Dirichlet condition $(L) = D$.

Using Galerkin's method, we multiply the differential equation by any $v \in V$ nd integrate terms with second-order derivatives by parts:

$$\int_0^L \alpha(u)u'v'\,\mathrm{d}x + \int_0^L auv\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x + [\alpha(u)u'v]_0^L, \quad \forall v \in V\,.$$

he Neumann condition at the boundary $x = 0$ is inserted in the boundary term:

$$[\alpha(u)u'v]_0^L = \alpha(u(L))u'(L)v(L) - \alpha(u(0))u'(0)v(0) = 0 - Cv(0) = -Cv(0)\,.$$

Recall that since $\psi_i(L) = 0$, any linear combination v of the basis functions also anishes at $x = L$: $v(L) = 0$.) The variational problem is then: find $u \in V$ such nat

$$\int_0^L \alpha(u)u'v'\,\mathrm{d}x + \int_0^L auv\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x - Cv(0), \quad \forall v \in V\,. \tag{51}$$

To derive the algebraic equations, we note that $\forall v \in V$ is equivalent with $= \psi_i$ for $i \in \mathcal{I}_s$. Setting $u = D + \sum_j c_j\psi_j$ and sorting terms results in the near system

$$\sum_{j\in\mathcal{I}_s}\left(\int_0^L \alpha(D + \sum_{k\in\mathcal{I}_s} c_k\psi_k)\psi_j'\psi_i'\,\mathrm{d}x\right)c_j = \int_0^L f(D+\sum_{k\in\mathcal{I}_s} c_k\psi_k)\psi_i\,\mathrm{d}x - C\psi_i(0), \quad i \in$$

(52)

undamental integration problem. Methods that use the Galerkin or eighted residual principle face a fundamental difficulty in nonlinear problems: ow can we integrate a terms like $\int_0^L \alpha(\sum_k c_k\psi_k)\psi_i'\psi_j'\,\mathrm{d}x$ and $\int_0^L f(\sum_k c_k\psi_k)\psi_i\,\mathrm{d}x$ hen we do not know the c_k coefficients in the argument of the α function? We an resort to numerical integration, provided an approximate $\sum_k c_k\psi_k$ can be sed for the argument u in f and α. If we want to derive the structure of the onlinear algebraic equations, we need to apply numerical integration based on ıe nodes only and/or the group finite element method.

.4 Finite element basis functions

ıtroduction of finite element basis functions φ_i means setting

$$\psi_i = \varphi_{\nu(i)}, \quad i \in \mathcal{I}_s,$$

where degree of freedom number $\nu(i)$ in the mesh corresponds to u number i (c_i). The expansion of u can still be

$$u = D + \sum_{j\in\mathcal{I}_s} c_j\varphi_{\nu(j)},$$

but is more common in a finite element context to use a boundary f $B = \sum_{j\in I_b} U_j\varphi_j$, where U_j are prescribed Dirichlet conditions for d freedom number j and U_j is the corresponding value. In the present e this means

$$u = D\varphi_0 + \sum_{j\in\mathcal{I}_s} c_j\varphi_{j+1}, \quad \mathcal{I}_s = \{0, \ldots, N_n - 2\}\,.$$

In the general case with u prescribed as U_j at some nodes $j \in I_b$, we se

$$u = \sum_{j\in I_b} U_j\varphi_j + \sum_{j\in\mathcal{I}_s} c_j\varphi_{\nu(j)},$$

where $c_j = u(x^{\nu(j)})$. That is, $\nu(j)$ maps unknown number j to the corres node number $\nu(j)$ such that $c_j = u(x^{\nu(j)})$.

4.5 The group finite element method

Finite element approximation of functions of u. Since we already u as $\sum_j \varphi_j u(x_j)$, we may use the same approximation for other func well. For example,

$$f(u) \approx \sum_j f(x_j)\varphi_j,$$

where $f(x_j)$ is the value of f at node j. Since f is a function of u, $f(u(x_j))$. Introducing u_j as a short form for $u(x_j)$, we can write

$$f(u) \approx \sum_j f(u_j)\varphi_j\,.$$

This approximation is known as the *group finite element method* or the *approximation* technique. The index j runs over all node numbers in th

The principal advantages of the group finite element method are tw

1. Complicated nonlinear expressions can be simplified to increase ciency of numerical computations.

2. One can derive *symbolic form* of the difference equations arising f finite element method in nonlinear problems. The symbolic form i for comparing finite element and finite difference equations of n differential equation problems.

elow, we shall explore point 2 to see exactly how the finite element method reates more complex expressions in the resulting linear system (the difference quations) that the finite difference method does. It turns out that is very difficult o see what kind of turns in the difference equations that arise from $\int f(u)\varphi_i\,\mathrm{d}x$ ithout using the group finite element method or numerical integration utilizing ne nodes only.

Note, however, that an expression like $\int f(u)\varphi_i\,\mathrm{d}x$ causes no problems in a omputer program as the integral is calculated by numerical integration using n existing approximation of u in $f(u)$ such that the integrand can be sampled t any spatial point.

implified problem. Our aim now is the derive symbolic expressions for the ifference equations arising from the finite element method in nonlinear problems nd compare the expressions with those arising in the finite difference method. o this, let us simplify the model problem and set $a = 0$, $\alpha = 1$, $f(u) = u^2$, and ave Neumann conditions at both ends such that we get a very simple nonlinear roblem $-u'' = u^2$, $u'(0) = 1$, $u'(L) = 0$. The variational form is then

$$\int_0^L u'v'\,\mathrm{d}x = \int_0^L u^2 v\,\mathrm{d}x - v(0), \quad \forall v \in V\,.$$

he term with $u'v'$ is well known so the only new feature is the term $\int u^2 v\,\mathrm{d}x$.

To make the distance from finite element equations to finite difference equaons as short as possible, we shall substitute c_j in the sum $u = \sum_j c_j\varphi_j$ by $_j = u(x_j)$ since c_j is the value of u at node j. (In the more general case with irichlet conditions as well, we have a sum $\sum_j c_j\varphi_{\nu(j)}$ where c_j is replaced by $(x_{\nu(j)})$. We can then introduce some other counter k such that it is meaningful write $u = \sum_k u_k\varphi_k$, where k runs over appropriate node numbers.) The uantity u_j in $\sum_j u_j\varphi_j$ is the same as u at mesh point number j in the finite ifference method, which is commonly denoted u_j.

ntegrating nonlinear functions. Consider the term $\int u^2 v\,\mathrm{d}x$ in the variaonal formulation with $v = \varphi_i$ and $u = \sum_k \varphi_k u_k$:

$$\int_0^L (\sum_k u_k\varphi_k)^2\varphi_i\,\mathrm{d}x\,.$$

valuating this integral for P1 elements (see Problem 11) results in the expression

$$\frac{h}{12}(u_{i-1}^2 + 2u_i(u_{i-1} + u_{i+1}) + 6u_i^2 + u_{i+1}^2),$$

be compared with the simple value u_i^2 that would arise in a finite difference iscretization when u^2 is sampled at mesh point x_i. More complicated $f(u)$ nctions give rise to much more lengthy expressions, if it is possible to carry ut the integral symbolically at all.

Application of the group finite element method. Let use the grou element method to derive the terms in the difference equation correspon $f(u)$ in the differential equation. We have

$$\int_0^L f(u)\varphi_i\,\mathrm{d}x \approx \int_0^L (\sum_j \varphi_j f(u_j))\varphi_i\,\mathrm{d}x = \sum_j \left(\int_0^L \varphi_i\varphi_j\,\mathrm{d}x\right) f(u_j$$

We recognize this expression as the mass matrix M, arising from $\int$ times the vector $f = (f(u_0), f(u_1), \ldots,)$: Mf. The associated terms difference equations are, for P1 elements,

$$\frac{h}{6}(f(u_{i-1}) + 4f(u_i) + f(u_{i+1}))\,.$$

Occasionally, we want to interpret this expression in terms of finite diff and to this end a rewrite of this expression is convenient:

$$\frac{h}{6}(f(u_{i-1}) + 4f(u_i) + f(u_{i+1})) = h[f(u) - \frac{h^2}{6}D_xD_xf(u)]_i\,.$$

That is, the finite element treatment of $f(u)$ (when using a group finite method) gives the same term as in a finite difference approach, $f(u_i)$, diffusion term which is the 2nd-order discretization of $\frac{1}{6}h^2 f''(x_i)$.

We may lump the mass matrix through integration with the Trapezoi so that M becomes diagonal in the finite element method. In that case t term in the differential equation gives rise to a single term $hf(u_i)$, just a finite difference method.

4.6 Numerical integration of nonlinear terms

Let us reconsider a term $\int f(u)v\,\mathrm{d}x$ as treated in the previous secti now we want to integrate this term numerically. Such an approach can easy-to-interpret formulas if we apply a numerical integration rule that the integrand at the node points x_i only, because at such points, $\varphi_j(x_$ $j \neq i$, which leads to great simplifications.

The term in question takes the form

$$\int_0^L f(\sum_k u_k\varphi_k)\varphi_i\,\mathrm{d}x\,.$$

Evaluation of the integrand at a node x_ℓ leads to a collapse of the sum $\sum$ to one term because

$$\sum_k u_k\varphi_k(x_\ell) = u_\ell\,.$$

$$f(\sum_k u_k \underbrace{\varphi_k(x_\ell)}_{\delta_{k\ell}})\underbrace{\varphi_i(x_\ell)}_{\delta_{i\ell}} = f(u_\ell)\delta_{i\ell},$$

here we have used the Kronecker delta: $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{ij} = 1$ if $i = j$.

Considering the Trapezoidal rule for integration, where the integration points re the nodes, we have

$$\int_0^L f(\sum_k u_k\varphi_k)(x)\varphi_i(x)\,\mathrm{d}x \approx h\sum_{\ell=0}^{N_n} f(u_\ell)\delta_{i\ell} - \mathcal{C} = hf(u_i)\,.$$

his is the same representation of the f term as in the finite difference method. he term $\mathcal{C}$ contains the evaluations of the integrand at the ends with weight $\frac{1}{2}$, eeded to make a true Trapezoidal rule:

$$\mathcal{C} = \frac{h}{2}f(u_0)\varphi_i(0) + \frac{h}{2}f(u_{N_n-1})\varphi_i(L)\,.$$

he answer $hf(u_i)$ must therefore be multiplied by $\frac{1}{2}$ if $i = 0$ or $i = N_n - 1$. ote that $\mathcal{C} = 0$ for $i = 1, \ldots, N_n - 2$.

One can alternatively use the Trapezoidal rule on the reference cell and ssemble the contributions. It is a bit more labor in this context, but working on ıe reference cell is safer as that approach is guaranteed to handle discontinuous erivatives of finite element functions correctly (not important in this particular xample), while the rule above was derived with the assumption that f is ontinuous at the integration points.

The conclusion is that it suffices to use the Trapezoidal rule if one wants o derive the difference equations in the finite element method and make them milar to those arising in the finite difference method. The Trapezoidal rule as sufficient accuracy for P1 elements, but for P2 elements one should turn to impson's rule.

.7 Finite element discretization of a variable coefficient Laplace term

urning back to the model problem (43), it remains to calculate the contribution f the $(\alpha u')'$ and boundary terms to the difference equations. The integral in ıe variational form corresponding to $(\alpha u')'$ is

$$\int_0^L \alpha(\sum_k c_k\psi_k)\psi_i'\psi_j'\,\mathrm{d}x\,.$$

umerical integration utilizing a value of $\sum_k c_k\psi_k$ from a previous iteration ıust in general be used to compute the integral. Now our aim is to integrate ymbolically, as much as we can, to obtain some insight into how the finite element ıethod approximates this term. To be able to derive symbolic expressions, we ıust either turn to the group finite element method or numerical integration in ıe node points. Finite element basis functions φ_i are now used.

Group finite element method. We set $\alpha(u) \approx \sum_k \alpha(u_k)\varphi_k$, and write

$$\int_0^L \alpha(\sum_k c_k\varphi_k)\varphi_i'\varphi_j'\,\mathrm{d}x \approx \sum_k (\underbrace{\int_0^L \varphi_k\varphi_i'\varphi_j'\,\mathrm{d}x}_{L_{i,j,k}})\alpha(u_k) = \sum_k L_{i,j,k}\alpha(u$$

Further calculations are now easiest to carry out in the reference cell. elements we can compute $L_{i,j,k}$ for the two k values that are relevant reference cell. Turning to local indices, one gets

$$L^{(e)}_{r,s,t} = \frac{1}{2h}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad t = 0, 1,$$

where $r, s, t = 0, 1$ are indices over local degrees of freedom in the refere $(i = q(e, r)$, $j = q(e, s)$, and $k = q(e, t))$. The sum $\sum_k L_{i,j,k}\alpha(u_k)$ at level becomes $\sum_{t=0}^{1} L^{(e)}_{r,s,t}\alpha(\tilde{u}_t)$, where $\tilde{u}_t$ is $u(x_{q(e,t)})$, i.e., the value of u node number t in cell number e. The element matrix becomes

$$\frac{1}{2}(\alpha(\tilde{u}_0) + \alpha(\tilde{u}^{(1)}))\frac{1}{h}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

As usual, we employ a left-to-right numbering of cells and nodes. Row n in the global matrix gets contributions from the first row of the element in cell $i - 1$ and the last row of the element matrix in cell i. In cell $i - 1$ the sum $\alpha(\tilde{u}_0) + \alpha(\tilde{u}^{(1)})$ corresponds to $\alpha(u_{i-1}) + \alpha(u_i)$. The sa becomes $\alpha(u_i) + \alpha(u_{i+1})$ in cell number i. We can with this insight a the contributions to row number i in the global matrix:

$$\frac{1}{2h}(-(\alpha(u_{i-1}) + \alpha(u_i)), \quad \alpha(u_{i-1}) + 2\alpha(u_i) + \alpha(u_{i+1}), \quad \alpha(u_i) + \alpha(u$$

Multiplying by the vector of unknowns u_i results in a formula that arranged to

$$-\frac{1}{h}(\frac{1}{2}(\alpha(u_i) + \alpha(u_{i+1}))(u_{i+1} - u_i) - \frac{1}{2}(\alpha(u_{i-1}) + \alpha(u_i))(u_i - u_{i-1})$$

which is nothing but the standard finite difference discretization of $-($ with an arithmetic mean of $\alpha(u)$ (and the usual factor h because of the int in the finite element method).

Numerical integration at the nodes. Instead of using the grou element method and exact integration we can turn to the Trapezoidal computing $\int_0^L \alpha(\sum_k u_k\varphi_k)\varphi_i'\varphi_j'\,\mathrm{d}x$, again at the cell level since that convenient when we deal with discontinuous functions φ_i':

$$\int_{-1}^{1} \alpha(\sum_t \tilde{u}_t\tilde{\varphi}_t)\tilde{\varphi}'_r\tilde{\varphi}'_s\frac{h}{2}dX = \int_{-1}^{1} \alpha(\sum_{t=0}^{1} \tilde{u}_t\tilde{\varphi}_t)\frac{2}{h}\frac{d\tilde{\varphi}_r}{dX}\frac{2}{h}\frac{d\tilde{\varphi}_s}{dX}\frac{h}{2}dX \tag{55}$$

$$= \frac{1}{2h}(-1)^r(-1)^s\int_{-1}^{1}\alpha(\sum_{t=0}^{1} u_t\tilde{\varphi}_t(X))dX$$

$$\approx \frac{1}{2h}(-1)^r(-1)^s\alpha(\sum_{t=0}^{1}\tilde{\varphi}_t(-1)\tilde{u}_t) + \alpha(\sum_{t=0}^{1}\tilde{\varphi}_t(1)\tilde{u}_t) = \frac{1}{2l}$$

(56)

The element matrix in (56) is identical to the one in (53), showing that the group finite element method and Trapezoidal integration are equivalent with a standard finite discretization of a nonlinear Laplace term $(\alpha(u)u')'$ using an arithmetic mean for α: $[D_x\overline{x}D_xu]_i$.

Remark about integration in the physical x coordinate.

We might comment on integration in the physical coordinate system too. The common Trapezoidal rule in Section 4.6 cannot be used to integrate derivatives like φ'_i, because the formula is derived under the assumption of a continuous integrand. One must instead use the more basic version of the Trapezoidal rule where all the trapezoids are summed up. This is straightforward, but I think it is even more straightforward to apply the Trapezoidal rule on the reference cell and assemble the contributions.

The term $\int auv\,\mathrm{d}x$ in the variational form is linear and gives these terms in the algebraic equations:

$$\frac{ah}{6}(u_{i-1} + 4u_i + u_{i+1}) = ah[u - \frac{h^2}{6}D_xD_xu]_i\,.$$

The final term in the variational form is the Neumann condition at the boundary: $Cv(0) = C\varphi_i(0)$. With a left-to-right numbering only $i = 0$ will give a contribution $Cv(0) = C\delta_{i0}$ (since $\varphi_i(0) \neq 0$ only for $i = 0$).

Summary.

For the equation

$$-(\alpha(u)u')' + au = f(u),$$

P1 finite elements results in difference equations where

- the term $-(\alpha(u)u')'$ becomes $-h[D_x\overline{\alpha(u)}^{x}D_xu]_i$ if the group element method or Trapezoidal integration is applied,
- $f(u)$ becomes $hf(u_i)$ with Trapezoidal integration or the "mass matrix" representation $h[f(u) - \frac{h}{6}D_xD_xf(u)]_i$ if computed by a g finite element method,
- au leads to the "mass matrix" form $ah[u - \frac{h}{6}D_xD_xu]_i$.

As we now have explicit expressions for the nonlinear difference eq also in the finite element method, a Picard or Newton method can be de shown for the finite difference method. However, our efforts in deriving s forms of the difference equations in the finite element method was motiva desire to see how nonlinear terms in differential equations make the finite and difference method different. For practical calculations in computer p we apply numerical integration, normally the more accurate Gauss-L quadrature rules, to the integrals directly. This allows us to easily *eval* nonlinear algebraic equations for a given numerical approximation of denoted u^-). To *solve* the nonlinear algebraic equations we need to ap Picard iteration method or Newton's method to the variational form dir shown next.

4.8 Picard iteration defined from the variational fo

We address again the problem (43) with the corresponding variational fo Our aim is to define a Picard iteration based on this variational form wit attempt to compute integrals symbolically as in the previous three sectio idea in Picard iteration is to use a previously computed u value in the n functions $\alpha(u)$ and $f(u)$. Let u^- be the available approximation to u f previous iteration. The linearized variational form for Picard iteration

$$\int_0^L (\alpha(u^-)u'v' + auv)\,\mathrm{d}x = \int_0^L f(u^-)v\,\mathrm{d}x - Cv(0), \quad \forall v \in V\,.$$

This is a linear problem $a(u, v) = L(v)$ with bilinear and linear forms

$$a(u,v) = \int_0^L (\alpha(u^-)u'v' + auv)\,\mathrm{d}x, \quad L(v) = \int_0^L f(u^-)v\,\mathrm{d}x - Cv(0$$

Make sure to distinguish the coefficient a in auv from the differential e from the a in the abstract bilinear form notation $a(\cdot,\cdot)$.

The linear system associated with (57) is computed the standard wa nically, we are back to solving $-(\alpha(x)u')' + au = f(x)$. The unknown u i on the form $u = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j$, with $B(x) = D$ and $\psi_i = \varphi_{\nu(i)}$, $\nu(i)$ and $\mathcal{I}_s = \{0, 1, \ldots, N = N_n - 2\}$.

.9 Newton's method defined from the variational form

pplication of Newton's method to the nonlinear variational form (51) arising om the problem (43) requires identification of the nonlinear algebraic equations $_i(c_0,\ldots,c_N)=0$, $i\in\mathcal{I}_s$, and the Jacobian $J_{i,j}=\partial F_i/\partial c_j$ for $i,j\in\mathcal{I}_s$.

The equations $F_i=0$ follows from the variational form

$$\int_0^L (\alpha(u)u'v' + auv)\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x - Cv(0), \quad \forall v\in V,$$

y choosing $v=\psi_i$, $i\in\mathcal{I}_s$, and setting $u=\sum_{j\in\mathcal{I}_s} c_j\psi_j$, maybe with a boundary nction to incorporate Dirichlet conditions.

With $v=\psi_i$ we get

$$F_i = \int_0^L (\alpha(u)u'\psi_i' + au\psi_i - f(u)\psi_i)\,\mathrm{d}x + C\psi_i(0) = 0, \quad i\in\mathcal{I}_s\,. \tag{58}$$

ı the differentiations leading to the Jacobian we will frequently use the results

$$\frac{\partial u}{\partial c_j} = \frac{\partial}{\partial c_j}\sum_k c_k\psi_k = \psi_j, \quad \frac{\partial u'}{\partial c_j} = \frac{\partial}{\partial c_j}\sum_k c_k\psi_k' = \psi_j'\,.$$

he derivation of the Jacobian of (58) goes as

$$\begin{aligned}
J_{i,j} = \frac{\partial F_i}{\partial c_j} &= \int_0^L \frac{\partial}{\partial c_j}(\alpha(u)u'\psi_i' + au\psi_i - f(u)\psi_i)\,\mathrm{d}x \\
&= \int_0^L ((\alpha'(u)\frac{\partial u}{\partial c_j}u' + \alpha(u)\frac{\partial u'}{\partial c_j})\psi_i' + a\frac{\partial u}{\partial c_j}\psi_i - f'(u)\frac{\partial u}{\partial c_j}\psi_i)\,\mathrm{d}x \\
&= \int_0^L ((\alpha'(u)\psi_j u' + \alpha(u)\psi_j'\psi_i' + a\psi_j\psi_i - f'(u)\psi_j\psi_i)\,\mathrm{d}x \\
&= \int_0^L (\alpha'(u)u'\psi_i'\psi_j + \alpha(u)\psi_i'\psi_j' + (a-f(u))\psi_i\psi_j)\,\mathrm{d}x
\end{aligned} \tag{59}$$

When calculating the right-hand side vector F_i and the coefficient matrix $_{i,j}$ in the linear system to be solved in each Newton iteration, one must use a reviously computed u, denoted by u^-, for the symbol u in (58) and (59). With ıis notation we have

$$F_i = \int_0^L \left(\alpha(u^-)u^{-\prime}\psi_i' + (a-f(u^-))\psi_i\right)\,\mathrm{d}x - C\psi_i(0), \quad i\in\mathcal{I}_s, \tag{60}$$

$$J_{i,j} = \int_0^L (\alpha'(u^-)u^{-\prime}\psi_i'\psi_j + \alpha(u^-)\psi_i'\psi_j' + (a-f(u^-))\psi_i\psi_j)\,\mathrm{d}x, \quad i,j\in\mathcal{I}_s\,. \tag{61}$$

These expressions can be used for any basis $\{\psi_i\}_{i\in\mathcal{I}_s}$. Choosing finite functions for ψ_i, one will normally want to compute the integral contribu by cell, working in a reference cell. To this end, we restrict the integratio cell and transform the cell to $[-1,1]$. The most recently computed approx u^- to u becomes $\tilde{u}^- = \sum_t \tilde{u}_t^{-1}\tilde{\varphi}_t(X)$ over the reference element, wher the value of u^- at global node (or degree of freedom) $q(e,t)$ correspondin local node t (or degree of freedom). The formulas (60) and (61) then ch

$$\tilde{F}_r^{(e)} = \int_{-1}^1 \left(\alpha(\tilde{u}^-)\tilde{u}^{-\prime}\tilde{\varphi}_r' + (a-f(\tilde{u}^-))\tilde{\varphi}_r\right)\det J\,\mathrm{d}X - C\tilde{\varphi}_r(0),$$

$$\tilde{J}_{r,s}^{(e)} = \int_{-1}^1 (\alpha'(\tilde{u}^-)\tilde{u}^{-\prime}\tilde{\varphi}_r'\tilde{\varphi}_s + \alpha(\tilde{u}^-)\tilde{\varphi}_r'\tilde{\varphi}_s' + (a-f(\tilde{u}^-))\tilde{\varphi}_r\tilde{\varphi}_s)\det J\,\mathrm{d}X$$

with $r,s\in I_d$ runs over the local degrees of freedom.

Many finite element programs require the user to provide F_i and $J_{i,}$ programs, like FEniCS[2], are capable of automatically deriving $J_{i,j}$ specified.

Dirichlet conditions. Incorporation of the Dirichlet values by ass contributions from all degrees of freedom and then modifying the linear can be obviously be applied to Picard iteration as that method involves a s linear system. In the Newton system, however, the unknown is a co δu to the solution. Dirichlet conditions are implemented by inserting the initial guess u^- for the Newton iteration and implementing $\delta u_i =$ known degrees of freedom. The manipulation of the linear system follows the algorithm in the linear problems, the only difference being that the values are zero.

5 Multi-dimensional PDE problems

5.1 Finite element discretization

The derivation of F_i and $J_{i,j}$ in the 1D model problem is easily genera multi-dimensional problems. For example, Backward Euler discretizatio PDE

$$u_t = \nabla\cdot(\alpha(u)\nabla u) + f(u),$$

gives the nonlinear time-discrete PDEs

$$u^n - \Delta t\nabla\cdot(\alpha(u^n)\nabla u^n) + f(u^n) = u^{n-1},$$

or with u^n simply as u and u^{n-1} as $u^{(1)}$,

[2] `http://fenicsproject.org`

$$u - \Delta t \nabla \cdot (\alpha(u^n)\nabla u) - \Delta t f(u) = u^{(1)}\,.$$

he variational form, assuming homogeneous Neumann conditions for simplicity, ecomes

$$\int_\Omega (uv + \Delta t \alpha(u)\nabla u \cdot \nabla v - \Delta t f(u)v - u^{(1)}v)\,\mathrm{d}x\,. \tag{65}$$

he nonlinear algebraic equations follow from setting $v = \psi_i$ and using the epresentation $u = \sum_k c_k\psi_k$, which we just write as

$$F_i = \int_\Omega (u\psi_i + \Delta t \alpha(u)\nabla u \cdot \nabla \psi_i - \Delta t f(u)\psi_i - u^{(1)}\psi_i)\,\mathrm{d}x\,. \tag{66}$$

icard iteration needs a linearization where we use the most recent approximation $^-$ to u in α and f:

$$F_i \approx \hat{F}_i = \int_\Omega (u\psi_i + \Delta t \alpha(u^-)\nabla u \cdot \nabla \psi_i - \Delta t f(u^-)\psi_i - u^{(1)}\psi_i)\,\mathrm{d}x\,. \tag{67}$$

he equations $\hat{F}_i = 0$ are now linear and we can easily derive a linear system for ie unknown coefficients $\{c_i\}_{i\in\mathcal{I}_s}$ by inserting $u = \sum_j c_j\psi_j$.

In Newton's method we need to evaluate F_i with the known value u^- for u:

$$F_i \approx \hat{F}_i = \int_\Omega (u^-\psi_i + \Delta t \alpha(u^-)\nabla u^- \cdot \nabla \psi_i - \Delta t f(u^-)\psi_i - u^{(1)}\psi_i)\,\mathrm{d}x\,. \tag{68}$$

he Jacobian is obtained by differentiating (66) and using $\partial u/\partial c_j = \psi_j$:

$$J_{i,j} = \frac{\partial F_i}{\partial c_j} = \int_\Omega (\psi_j\psi_i + \Delta t \alpha'(u)\psi_j\nabla u \cdot \nabla\psi_i + \Delta t\alpha(u)\nabla\psi_j \cdot \nabla\psi_i - \Delta t f'(u)\psi_j\psi_i)\,\mathrm{d}x\,. \tag{69}$$

he evaluation of $J_{i,j}$ as the coefficient matrix in the linear system in Newton's ıethod applies the known approximation u^- for u:

$$J_{i,j} = \int_\Omega (\psi_j\psi_i + \Delta t \alpha'(u^-)\psi_j\nabla u^- \cdot \nabla\psi_i + \Delta t\alpha(u^-)\nabla\psi_j \cdot \nabla\psi_i - \Delta t f'(u^-)\psi_j\psi_i)\,\mathrm{d}x\,. \tag{70}$$

opefully, these example also show how convenient the notation with u and $^-$ is: the unknown to be computed is always u and linearization by inserting nown (previously computed) values is a matter of adding an underscore. One ın take great advantage of this quick notation in software [2].

Non-homogeneous Neumann conditions. A natural physical flu tion for the PDE (64) takes the form of a non-homogeneous Neumann c

$$-\alpha(u)\frac{\partial u}{\partial n} = g, \quad \boldsymbol{x} \in \partial\Omega_N,$$

where g is a prescribed function and $\partial\Omega_N$ is a part of the boundary of the Ω. From integrating $\int_\Omega \nabla\cdot(\alpha\nabla u)\,\mathrm{d}x$ by parts, we get a boundary term

$$\int_{\partial\Omega_N} \alpha(u)\frac{\partial u}{\partial u}v\,\mathrm{d}s\,.$$

Inserting the condition (71) into this term results in an integral over pr values: $-\int_{\partial\Omega_N} gv\,\mathrm{d}s$. The nonlinearity in the $\alpha(u)$ coefficient condit therefore does not contribute with a nonlinearity in the variational forı

Robin conditions. Heat conduction problems often apply a kind of N cooling law, also known as a Robin condition, at the boundary:

$$-\alpha(u)\frac{\partial u}{\partial u} = h_T(u)(u - T_s(t)), \quad \boldsymbol{x} \in \partial\Omega_R,$$

where $h_T(u)$ is a heat transfer coefficient between the body (Ω) and roundings, T_s is the temperature of the surroundings, and $\partial\Omega_R$ is a paı boundary where this Robin condition applies. The boundary integral (becomes

$$\int_{\partial\Omega_R} h_T(u)(u - T_s(T))v\,\mathrm{d}s,$$

by replacing $\alpha(u)\partial u/\partial u$ by $h_T(u - T_s)$. Often, $h_T(u)$ can be taken as c and then the boundary term is linear in u, otherwise it is nonlinear and con to the Jacobian in a Newton method. Linearization in a Picard metl typically use a known value in h_T, but keep the u in $u - T_s$ as u $h_T(u^-)(u - T_s(t))$.

5.2 Finite difference discretization

A typical diffusion equation

$$u_t = \nabla\cdot(\alpha(u)\nabla u) + f(u),$$

can be discretized by (e.g.) a Backward Euler scheme, which in 2D written

$$[D_t^- u = D_x\overline{\alpha}^x D_x u + D_y\overline{\alpha}^y D_y u + f(u)]^n_{i,j}\,.$$

We do not dive into details of boundary conditions now. Dirichlet and N conditions are handled as in linear diffusion problems.

Writing the scheme out, putting the unknown values on the left-hand side nd known values on the right-hand side, and introducing $\Delta x = \Delta y = h$ to save ome writing, one gets

$$
\begin{aligned}
u^n_{i,j} - \frac{\Delta t}{h^2}(&\frac{1}{2}(\alpha(u^n_{i,j}) + \alpha(u^n_{i+1,j}))(u^n_{i+1,j} - u^n_{i,j}) \\
&- \frac{1}{2}(\alpha(u^n_{i-1,j}) + \alpha(u^n_{i,j}))(u^n_{i,j} - u^n_{i-1,j}) \\
&+ \frac{1}{2}(\alpha(u^n_{i,j}) + \alpha(u^n_{i,j+1}))(u^n_{i,j+1} - u^n_{i,j}) \\
&- \frac{1}{2}(\alpha(u^n_{i,j-1}) + \alpha(u^n_{i,j}))(u^n_{i,j} - u^n_{i-1,j-1})) - \Delta t f(u^n_{i,j}) = u^{n-1}_{i,j}
\end{aligned}
$$

his defines a nonlinear algebraic system $A(u)u = b(u)$. A Picard iteration pplies old values u^- in α and f, or equivalently, old values for u in $A(u)$ and (u). The result is a linear system of the same type as those arising from $_t = \nabla \cdot (\alpha(\boldsymbol{x})\nabla u) + f(\boldsymbol{x}, t)$.

Newton's method is as usual more involved. We first define the nonlinear lgebraic equations to be solved, drop the superscript n, and introduce $u^{(1)}$ for $^{n-1}$:

$$
\begin{aligned}
{}_{i,j} = u^n_{i,j} - \frac{\Delta t}{h^2}(&\\
&\frac{1}{2}(\alpha(u^n_{i,j}) + \alpha(u^n_{i+1,j}))(u^n_{i+1,j} - u^n_{i,j}) - \frac{1}{2}(\alpha(u^n_{i-1,j}) + \alpha(u^n_{i,j}))(u^n_{i,j} - u^n_{i-1,j}) + \\
&\frac{1}{2}(\alpha(u^n_{i,j}) + \alpha(u^n_{i,j+1}))(u^n_{i,j+1} - u^n_{i,j}) - \frac{1}{2}(\alpha(u^n_{i,j-1}) + \alpha(u^n_{i,j}))(u^n_{i,j} - u^n_{i-1,j-1})) \\
&\Delta t f(u^n_{i,j}) - u^{n-1}_{i,j} = 0\,.
\end{aligned}
$$

is convenient to work with two indices i and j in 2D finite difference discretizaons, but it complicates the derivation of the Jacobian, which then gets four ndices. The left-hand expression of an equation $F_{i,j} = 0$ is to be differentiated ith respect to each of the unknowns $u_{r,s}$ (short for $u^n_{r,s}$), $r \in \mathcal{I}_x$, $s \in \mathcal{I}_y$,

$$
J_{i,j,r,s} = \frac{\partial F_{i,j}}{\partial u_{r,s}}\,.
$$

iven i and j, only a few r and s indices give nonzero contribution since $F_{i,j}$ ontains $u_{i\pm1,j}$, $u_{i,j\pm1}$, and $u_{i,j}$. Therefore, $J_{i,j,r,s}$ is very sparse and we can set p the left-hand side of the Newton system as

$$
\begin{aligned}
{}_{i,j,r,s}\delta u_{r,s} = J_{i,j,i,j}\delta u_{i,j} + J_{i,j,i-1,j}\delta u_{i-1,j} + J_{i,j,i+1,j}\delta u_{i+1,j} + J_{i,j,i,j-1}\delta u_{i,j-1} \\
+ J_{i,j,i,j+1}\delta u_{i,j+1}
\end{aligned}
$$

he specific derivatives become

$$
\begin{aligned}
J_{i,j,i-1,j} &= \frac{\partial F_{i,j}}{\partial u_{i-1,j}} \\
&= \frac{\Delta t}{h^2}(\alpha'(u_{i-1,j})(u_{i,j} - u_{i-1,j}) + \alpha(u_{i-1,j})(-1)) \\
J_{i,j,i+1,j} &= \frac{\partial F_{i,j}}{\partial u_{i+1,j}} \\
&= \frac{\Delta t}{h^2}(-\alpha'(u_{i+1,j})(u_{i+1,j} - u_{i,j}) - \alpha(u_{i-1,j})) \\
J_{i,j,i,j-1} &= \frac{\partial F_{i,j}}{\partial u_{i,j-1}} \\
&= \frac{\Delta t}{h^2}(\alpha'(u_{i,j-1})(u_{i,j} - u_{i,j-1}) + \alpha(u_{i,j-1})(-1)) \\
J_{i,j,i,j+1} &= \frac{\partial F_{i,j}}{\partial u_{i,j+1}} \\
&= \frac{\Delta t}{h^2}(-\alpha'(u_{i,j+1})(u_{i,j+1} - u_{i,j}) - \alpha(u_{i,j-1}))
\end{aligned}
$$

The $J_{i,j,i,j}$ entry has a few more terms. Inserting u^- for u in the J form then forming $J\delta u = -F$ gives the linear system to be solved in each iteration.

5.3 Continuation methods

Picard iteration or Newton's method may diverge when solving PDEs wit nonlinearities. Relaxation with $\omega < 1$ may help, but in highly nonlinear p it can be necessary to introduce a *continuation parameter* Λ in the p $\Lambda = 0$ gives a version of the problem that is easy to solve, while $\Lambda = 1$ is th problem. The idea is then to increase Λ in steps, $\Lambda_0 = 0, \Lambda_1 < \cdots < \Lambda_n =$ use the solution from the problem with Λ_{i-1} as initial guess for the itera the problem corresponding to Λ_i.

The continuation method is easiest to understand through an e Suppose we intend to solve

$$
-\nabla \cdot (||\nabla u||^q \nabla u) = f,
$$

which is an equation modeling the flow of a non-Newtonian fluid th channel or pipe. For $q = 0$ we have the Poisson equation (correspond Newtonian fluid) and the problem is linear. A typical value for pseudo fluids may be $q_n = -0.8$. We can introduce the continuation parameter Λ such that $q = q_n\Lambda$. Let $\{\Lambda_\ell\}_{\ell=0}^n$ be the sequence of Λ values in $[0,$ corresponding q values $\{q_\ell\}_{\ell=0}^n$. We can then solve a sequence of proble

$$
-\nabla \cdot \left(||\nabla u||_\ell^q \nabla u^\ell\right) = f, \quad \ell = 0, \ldots, n,
$$

here the initial guess for iterating on u^ℓ is the previously computed solution $^{\ell-1}$. If a particular Λ_ℓ leads to convergence problems, one may try a smaller ıcrease in Λ: $\Lambda_* = \frac{1}{2}(\Lambda_{\ell-1} + \Lambda_\ell)$, and repeat halving the step in Λ until ɔnvergence is reestablished.

Exercises

roblem 1: Determine if equations are nonlinear or not

lassify each term in the following equations as linear or nonlinear. Assume that and b are unknown numbers and that u and v are unknown functions. All ther symbols are known quantities.

1. $b^2 = 1$
2. $a + b = 1$, $a - 2b = 0$
3. $mu'' + \beta|u'|u' + cu = F(t)$
4. $u_t = \alpha u_{xx}$
5. $u_{tt} = c^2\nabla^2 u$
6. $u_t = \nabla \cdot (\alpha(u)\nabla u) + f(x, y)$
7. $u_t + f(u)_x = 0$
8. $\boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + r\nabla^2 \boldsymbol{u}$, $\nabla \cdot \boldsymbol{u} = 0$ ($\boldsymbol{u}$ is a vector field)
9. $u' = f(u, t)$
10. $\nabla^2 u = \lambda e^u$

xercise 2: Derive a formula

erive (9) in Section 1.7. Filename: `relaxed_Newton.pdf`.

roblem 3: Experience the behavior of Newton's method

he program `Newton_demo.py`[3] illustrates graphically each step in Newton's ıethod and is run like

```
erminal> python Newton_demo.py f dfdx x0 xmin xmax
```

[3] `http://tinyurl.com/nm5587k/nonlin/Newton_demo.py`

Use this program to investigate potential problems with Newton's metho solving $e^{-0.5x^2}\cos(\pi x) = 0$. Try a starting point $x_0 = 0.8$ and $x_0 = 0$ watch the different behavior. Just run

```
Terminal>  python Newton_demo.py '0.2 + exp(-0.5*x**2)*cos(pi*x)'
           '-x*exp(-x**2)*cos(pi*x) - pi*exp(-x**2)*sin(pi*x)' \
           0.85 -3 3
```

and repeat with 0.85 replaced by 0.8.

Problem 4: Linearize a nonlinear vibration ODE

Consider a nonlinear vibration problem

$$mu'' + bu'|u'| + s(u) = F(t),$$

where $m > 0$ is a constant, $b \geq 0$ is a constant, $s(u)$ a possibly nonlinear f of u, and $F(t)$ is a prescribed function. Such models arise from Newton's law of motion in mechanical vibration problems where $s(u)$ is a spring or r force, mu'' is mass times acceleration, and $bu'|u'|$ models water or air d

Rewrite the equation for u as a system of two first-order ODEs, and d this system by a Crank-Nicolson (centered difference) method. With we get a nonlinear term $v^{n+\frac{1}{2}}|v^{n+\frac{1}{2}}|$. Use both a geometric and an ari average for $v^{n+\frac{1}{2}}$. In the latter case, explain how to apply Newton's me solve the nonlinear equations at each time level.

Exercise 5: Find the sparsity of the Jacobian

Consider a typical nonlinear Laplace term like $\nabla\cdot\alpha(u)\nabla u$ discretized by c finite differences. Explain why the Jacobian corresponding to this term same sparsity pattern as the matrix associated with the correspondin term $\alpha\nabla^2 u$.

Hint. Set up the unknowns that enter the difference stencil and f sparsity of the Jacobian that arise from the stencil.
Filename: `nonlin_sparsity_Jacobian.pdf`.

Exercise 6: Newton's method for linear problems

Suppose we have a linear system $F(u) = Au - b = 0$. Apply Newton's to this system, and show that the method converges in one iteration. F `nonlin_Newton_linear.pdf`.

Exercise 7: Differentiate a highly nonlinear term

The operator $\nabla \cdot (\alpha(u)\nabla u)$ with $\alpha(u) = ||\nabla u||^q$ appears in several physical problems, especially flow of Non-Newtonian fluids. In a Newton method one has to carry out the differentiation $\partial\alpha(u)/\partial c_j$, for $u = \sum_k c_k\psi_k$. Show that

$$\frac{\partial}{\partial u_j}||\nabla u||^q = q||\nabla u||^{q-2}\nabla u \cdot \nabla\psi_j \,.$$

Filename: `nonlin_differentiate.pdf`.

Problem 8: Discretize a 1D problem with a nonlinear coefficient

We consider the problem

$$((1+u^2)u')' = 1, \quad x \in (0,1), \quad u(0) = u(1) = 0\,. \tag{75}$$

a) Discretize (75) by a centered finite difference method on a uniform mesh.

b) Discretize (75) by a finite element method with P1 of equal length. Use the Trapezoidal method to compute all integrals. Set up the resulting matrix system.
Filename: `nonlin_1D_coeff_discretize.pdf`.

Problem 9: Linearize a 1D problem with a nonlinear coefficient

We have a two-point boundary value problem

$$((1+u^2)u')' = 1, \quad x \in (0,1), \quad u(0) = u(1) = 0\,. \tag{76}$$

a) Construct a Picard iteration method for (76) without discretizing in space.

b) Apply Newton's method to (76) without discretizing in space.

c) Discretize (76) by a centered finite difference scheme. Construct a Picard method for the resulting system of nonlinear algebraic equations.

d) Discretize (76) by a centered finite difference scheme. Define the system of nonlinear algebraic equations, calculate the Jacobian, and set up Newton's method for solving the system.
Filename: `nonlin_1D_coeff_linearize.pdf`.

Problem 10: Finite differences for the 1D Bratu prob

We address the so-called Bratu problem

$$u'' + \lambda e^u = 0, \quad x \in (0,1), \quad u(0) = u(1) = 0,$$

where λ is a given parameter and u is a function of x. This is a widely used problem for studying numerical methods for nonlinear differential eq The problem (77) has an exact solution

$$u(x) = -2\ln\left(\frac{\cosh((x-\frac{1}{2})\theta/2)}{\cosh(\theta/4)}\right),$$

where θ solves

$$\theta = \sqrt{2\lambda}\cosh(\theta/4)\,.$$

There are two solutions of (77) for $0 < \lambda < \lambda_c$ and no solution for $\lambda > \lambda = \lambda_c$ there is one unique solution. The critical value λ_c solves

$$1 = \sqrt{2\lambda_c}\frac{1}{4}\sinh(\theta(\lambda_c)/4)\,.$$

A numerical value is $\lambda_c = 3.513830719$.

a) Discretize (77) by a centered finite difference method.

b) Set up the nonlinear equations $F_i(u_0, u_1, \ldots, u_{N_x}) = 0$ from a). C the associated Jacobian.
Filename: `nonlin_1D_Bratu_fd.pdf`.

Problem 11: Integrate functions of finite element e sions

We shall investigate integrals on the form

$$\int_0^L f(\sum_k u_k\varphi_k(x))\varphi_i(x)\,\mathrm{d}x,$$

where $\varphi_i(x)$ are P1 finite element basis functions and u_k are unknown coe more precisely the values of the unknown function u at nodes x_k. We intr node numbering that goes from left to right and also that all cells have t length h. Given i, the integral only gets contributions from $[x_{i-1}, x_{i+1}]$. interval $\varphi_k(x) = 0$ for $k < i-1$ and $k > i+1$, so only three basis functi contribute:

$$\sum_k u_k\varphi_k(x) = u_{i-1}\varphi_{i-1}(x) + u_i\varphi_i(x) + u_{i+1}\varphi_{i+1}(x)\,.$$

The integral (78) now takes the simplified form

$$\int_{x_{i-1}}^{x_{i+1}} f(u_{i-1}\varphi_{i-1}(x) + u_i\varphi_i(x) + u_{i+1}\varphi_{i+1}(x))\varphi_i(x)\,\mathrm{d}x\,.$$

plit this integral in two integrals over cell L (left), $[x_{i-1}, x_i]$, and cell R (right), $_i, x_{i+1}]$. Over cell L, u simplifies to $u_{i-1}\varphi_{i-1} + u_i\varphi_i$ (since $\varphi_{i+1} = 0$ on this ell), and over cell R, u simplifies to $u_i\varphi_i + u_{i+1}\varphi_{i+1}$. Make a `sympy` program hat can compute the integral and write it out as a difference equation. Give he $f(u)$ formula on the command line. Try out $f(u) = u^2, \sin u, \exp u$.

lint. Introduce symbols `u_i`, `u_im1`, and `u_ip1` for u_i, u_{i-1}, and u_{i+1}, re-pectively, and similar symbols for x_i, x_{i-1}, and x_{i+1}. Find formulas for the asis functions on each of the two cells, make expressions for u on the two cells, ntegrate over each cell, expand the answer and simplify. You can make LaTeX ode and render it via `http://latex.codecogs.com`. Here are some appropriate ython statements for the latter purpose:

```
rom sympy import *
...
# expr_i holdes the integral as a sympy expression
latex_code = latex(expr_i, mode='plain')
# Replace u_im1 sympy symbol name by latex symbol u_{i-1}
latex_code = latex_code.replace('im1', '{i-1}')
# Replace u_ip1 sympy symbol name by latex symbol u_{i+1}
latex_code = latex_code.replace('ip1', '{i+1}')
# Escape (quote) latex_code so it can be sent as HTML text
import cgi
tml_code = cgi.escape(latex_code)
# Make a file with HTML code for displaying the LaTeX formula
 = open('tmp.html', 'w')
# Include an image that can be clicked on to yield a new
# page with an interactive editor and display area where the
# formula can be further edited
ext = """
<a href="http://www.codecogs.com/eqnedit.php?latex=%(html_code)s"
 target="_blank">
<img src="http://latex.codecogs.com/gif.latex?%(html_code)s"
 title="%(latex_code)s"/>
</a>
 """ % vars()
.write(text)
.close()
```

he formula is displayed by loading `tmp.html` into a web browser.
ilename: `fu_fem_int.py`.

roblem 12: Finite elements for the 1D Bratu problem

/e address the same 1D Bratu problem as described in Problem 10.

) Discretize (12) by a finite element method using a uniform mesh with P1 ements. Use a group finite element method for the e^u term.

b) Set up the nonlinear equations $F_i(u_0, u_1, \ldots, u_{N_x}) = 0$ from a). C the associated Jacobian.
Filename: `nonlin_1D_Bratu_fe.pdf`.

Problem 13: Derive the Newton system from a varia form

We study the multi-dimensional heat conduction PDE

$$\varrho c(T)T_t = \nabla\cdot(k(T)\nabla T)$$

in a spatial domain Ω, with a nonlinear Robin boundary condition

$$-k(T)\frac{\partial T}{\partial n} = h(T)(T - T_s(t)),$$

at the boundary $\partial\Omega$. The primary unknown is the temperature T, ϱ is the of the solid material, $c(T)$ is the heat capacity, $k(T)$ is the heat conducti is a heat transfer coefficient, and $T_s(T)$ is a possibly time-dependent tem of the surroundings.

a) Use a Backward Euler or Crank-Nicolson time discretization and de variational form for the spatial problem to be solved at each time level.

b) Define a Picard iteration method from the variational form at a tim

c) Derive expressions for the matrix and the right-hand side of the e system that arises from applying Newton's method to the variational fo time level.

d) Apply the Backward Euler or Crank-Nicolson scheme in time first. a Newton method at the PDE level. Make a variational form of the r PDE at a time level.
Filename: `nonlin_heat_Newton.pdf`.

Problem 14: Derive algebraic equations for nonline heat conduction

Consider a 1D heat conduction PDE

$$\varrho c(T)T_t = (k(T)T_x)_x,$$

where ϱ is the density of the solid material, $c(T)$ is the heat capacity, temperature, and $k(T)$ is the heat conduction coefficient.

Use a uniform finite element mesh, P1 elements, and the group finite method to derive the algebraic equations arising from the heat conducti

a) Discretize the PDE by a finite difference method. Use either a Ba Euler or Crank-Nicolson scheme in time.

) Derive the matrix and right-hand side of a Newton method applied to the iscretized PDE.
ilename: `nonlin_1D_heat_PDE.pdf`.

'roblem 15: Investigate a 1D problem with a continuation ıethod

low of a pseudo-plastic power-law fluid between two flat plates can be modeled y

$$\frac{d}{dx}\left(\mu_0\left|\frac{du}{dx}\right|^{n-1}\frac{du}{dx}\right) = -\beta, \quad u'(0) = 0,\ u(H) = 0,$$

here $\beta > 0$ and $\mu_0 > 0$ are constants. A target value of n may be $n = 0.2$.

) Formulate a Picard iteration method directly for the differential equation roblem.

) Perform a finite difference discretization of the problem in each Picard eration. Implement a solver that can compute u on a mesh. Verify that the olver gives an exact solution for $n = 1$ on a uniform mesh regardless of the cell ze.

) Given a sequence of decreasing n values, solve the problem for each n sing the solution for the previous n as initial guess for the Picard iteration. his is called a continuation method. Experiment with $n = (1, 0.6, 0.2)$ and $= (1, 0.9, 0.8, \ldots, 0.2)$ and make a table of the number of Picard iterations ersus n.

) Derive a Newton method at the differential equation level and discretize the esulting linear equations in each Newton iteration with the finite difference ıethod.

) Investigate if Newton's method has better convergence properties than Picard eration, both in combination with a continuation method.

Leferences

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